

AN ADAPTIVE FINITE ELEMENT PML METHOD FOR THE ELASTIC WAVE SCATTERING PROBLEM IN PERIODIC STRUCTURES

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ABSTRACT. An adaptive finite element method is presented for the elastic scattering of a time-harmonic plane wave by a periodic surface. First, the unbounded physical domain is truncated into a bounded computational domain by introducing the perfectly matched layer (PML) technique. The well-posedness and exponential convergence of the solution are established for the truncated PML problem by developing an equivalent transparent boundary condition. Second, an a posteriori error estimate is deduced for the discrete problem and is used to determine the finite elements for refinements and to determine the PML parameters. Numerical experiments are included to demonstrate the competitive behavior of the proposed adaptive method.

1. INTRODUCTION

The scattering theory in periodic diffractive structures, which are known as diffraction gratings, has many significant applications in optical industry [7, 8]. The time-harmonic problems have been studied extensively in diffraction gratings by many researchers for acoustic, electromagnetic, and elastic waves [1, 2, 4, 5, 15, 22–24, 29, 32]. The underlying equations of these waves are the Helmholtz equation, the Maxwell equations, and the Navier equation, respectively. This paper is concerned with the numerical solution of the elastic wave scattering problem in such a periodic structure. The problem has two fundamental challenges. The first one is to truncate the unbounded physical domain into a bounded computational domain. The second one is the singularity of the solution due to nonsmooth grating surfaces. Hence, the goal of this work is two fold to overcome these two issues. First, we adopt the perfectly matched layer (PML) technique to handle the domain truncation. Second, we use an a posteriori error analysis and design a finite element method with adaptive mesh refinements to deal with the singularity of the solution.

The research on the PML technique has undergone a tremendous development since Bérenger proposed a PML for solving the time-dependent Maxwell equations [11]. The basis idea of the PML technique is to surround the domain of interest by a layer of finite thickness fictitious material which absorbs all the waves coming from inside the computational domain. When the waves reach the outer boundary of the PML region, their energies are so small that the simple homogeneous Dirichlet boundary conditions can be imposed. Various constructions of PML absorbing layers have been proposed and investigated for the acoustic and electromagnetic wave scattering problems [10, 12, 19–21, 27, 28, 31]. The PML technique is much less studied for the elastic wave scattering problems [25], especially for the rigorous convergence analysis. We refer to [13, 18] for recent study on convergence analysis of the elastic obstacle scattering problem. Combined with the PML technique, an effective adaptive finite element method was proposed in [6, 16] to solve the two-dimensional diffraction grating problem where the one-dimensional grating structure was considered. Due to the competitive numerical performance, the method was quickly adopted to solve many other scattering problems including the obstacle scattering problems [14, 17] and the three-dimensional diffraction grating problem [9]. Based on the a posteriori error analysis, the adaptive finite element PML method provides an

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effective numerical strategy which can be used to solve a variety of wave propagation problems which are imposed in unbounded domains.

In this paper, we explore the possibility of applying such an adaptive finite element PML method to solve the diffraction grating problem of elastic waves. Specifically, we consider the incidence of a time-harmonic elastic plane wave on a one-dimensional grating surface, which is assumed to be elastically rigid. The open space, which is above the surface, is assumed to be filled with a homogeneous and isotropic elastic medium. Using the quasi-periodicity of the solution and the transparent boundary condition, we formulate the scattering problem equivalently into a boundary value problem in a bounded domain. The conservation of energy is proved for the model problem and is used to verify our numerical results when the exact solutions are not available. Following the complex coordinate stretching, we study the truncated PML problem which is an approximation to the original scattering problem. We develop the transparent boundary condition for the truncated PML problem and show that it has a unique weak solution which converges exponentially to the solution of the original scattering problem. Moreover, an a posteriori error estimate is deduced for the discrete PML problem. It consists of the finite element error and the PML modeling error. The estimate is used to design the adaptive finite element algorithm to choose elements for refinements and to determine the PML parameters. Numerical experiments show that the proposed method can effectively overcome the aforementioned two challenges.

This paper presents a nontrivial application of the adaptive finite element PML method for the grating problem from the Helmholtz (acoustic) and Maxwell (electromagnetic) equations to the Navier (elastic) equation. The elastic wave equation is complicated due to the coexistence of compressional and shear waves that have different wavenumbers and propagate at different speeds. In view of this physical feature, we introduce two scalar potential functions to split the wave field into its compressional and shear parts via the Helmholtz decomposition. As a consequence, the analysis is much more sophisticated than that for the Helmholtz equation or the Maxwell equations. We believe that this work not only enriches the range of applications for the PML technique but also is a valued contribution to the family of numerical methods for solving elastic wave scattering problems.

The paper is organized as follows. In section 2, we introduce the model problem of the elastic wave scattering by a periodic surface and formulate it into a boundary value problem by using a transparent boundary condition. The conservation of the total energy is proved for the propagating wave modes. In section 3, we introduce the PML formulation and prove the well-posedness and convergence of the truncated PML problem. Section 4 is devoted to the finite element approximation and the a posteriori error estimate. In section 5, we discuss the numerical implementation of our adaptive algorithm and present some numerical experiments to illustrate the performance of the proposed method. The paper is concluded with some general remarks and directions for future research in section 6.

2. PROBLEM FORMULATION

In this section, we introduce the model problem and present an exact transparent boundary condition to reduce the problem into a boundary value problem in a bounded domain. The energy distribution will be studied for the reflected propagating waves of the scattering problem.

2.1. Navier equation. Consider the elastic scattering of a time-harmonic plane wave by a periodic surface S which is assumed to be Lipschitz continuous and elastically rigid. In this work, we consider the two-dimensional problem by assuming that the surface is invariant in the z direction. The three-dimensional problem will be studied as a separate work. Figure 1 shows the problem geometry in one period. Let $\mathbf{x} = [x, y]^T \in \mathbb{R}^2$. Denote by $\Gamma = \{\mathbf{x} \in \mathbb{R}^2 : 0 < x < \Lambda, y = b\}$ the artificial boundary above the scattering surface, where Λ is the period and b is a constant. Let Ω be the bounded domain which is enclosed from below and above by S and Γ , respectively. Finally, denote by $\Omega^e = \{\mathbf{x} \in \mathbb{R}^2 : 0 < x < \Lambda, y > b\}$ the exterior domain to Ω .

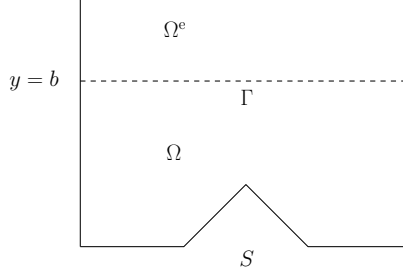


FIGURE 1. Geometry of the scattering problem.

The open space, which is above the grating surface, is assumed to be filled with a homogeneous and isotropic elastic medium with a unit mass density. The propagation of a time-harmonic elastic wave is governed by the Navier equation

$$\mu \Delta \mathbf{u} + (\lambda + \mu) \nabla \nabla \cdot \mathbf{u} + \omega^2 \mathbf{u} = 0 \quad \text{in } \Omega \cup \Omega^e, \quad (2.1)$$

where $\omega > 0$ is the angular frequency, μ and λ are the Lamé constants satisfying $\mu > 0$ and $\lambda + \mu > 0$, and $\mathbf{u} = [u_1, u_2]^\top$ is the displacement vector of the total field which satisfies

$$\mathbf{u} = 0 \quad \text{on } S. \quad (2.2)$$

Let the surface be illuminated from above by either a time-harmonic compressional plane wave

$$\mathbf{u}_{\text{inc}}(\mathbf{x}) = [\sin \theta, -\cos \theta]^\top e^{i\kappa_1(x \sin \theta - y \cos \theta)},$$

or a time-harmonic shear plane wave

$$\mathbf{u}_{\text{inc}}(\mathbf{x}) = [\cos \theta, \sin \theta]^\top e^{i\kappa_2(x \sin \theta - y \cos \theta)},$$

where $\theta \in (-\pi/2, \pi/2)$ is the incident angle and

$$\kappa_1 = \frac{\omega}{\sqrt{\lambda + 2\mu}}, \quad \kappa_2 = \frac{\omega}{\sqrt{\mu}} \quad (2.3)$$

are the compressional and shear wavenumbers, respectively. It can be verified that the incident wave also satisfies the Navier equation:

$$\mu \Delta \mathbf{u}_{\text{inc}} + (\lambda + \mu) \nabla \nabla \cdot \mathbf{u}_{\text{inc}} + \omega^2 \mathbf{u}_{\text{inc}} = 0 \quad \text{in } \Omega \cup \Omega^e. \quad (2.4)$$

Remark 2.1. *Our method works for either the compressional plane incident wave, or the shear plane incident wave, or any linear combination of these two plane incident waves. For clarity, we will take the compressional plane incident wave as an example to present the results in our subsequent analysis.*

Motivated by uniqueness, we are interested in a quasi-periodic solution of \mathbf{u} , i.e., $\mathbf{u}(x, y)e^{-i\alpha x}$ is periodic in x with period Λ where $\alpha = \kappa_1 \sin \theta$. In addition, the following radiation condition is imposed: the total displacement \mathbf{u} consists of bounded outgoing waves plus the incident wave \mathbf{u}_{inc} in Ω^e .

We introduce some notation and Sobolev spaces. Let $\mathbf{u} = [u_1, u_2]^\top$ and u be a vector and scalar function, respectively. Define the Jacobian matrix of \mathbf{u} as

$$\nabla \mathbf{u} = \begin{bmatrix} \partial_x u_1 & \partial_y u_1 \\ \partial_x u_2 & \partial_y u_2 \end{bmatrix}$$

and two curl operators

$$\text{curl} \mathbf{u} = \partial_x u_2 - \partial_y u_1, \quad \mathbf{curl} u = [\partial_y u, -\partial_x u]^\top.$$

Define a quasi-periodic functional space

$$H_{S, \text{qp}}^1(\Omega) = \{u \in H^1(\Omega) : u(\Lambda, y) = u(0, y)e^{i\alpha\Lambda}, u = 0 \text{ on } S\},$$

which is a subspace of $H^1(\Omega)$ with the norm $\|\cdot\|_{H^1(\Omega)}$. For any quasi-periodic function u defined on Γ , it admits the Fourier series expansion

$$u(x) = \sum_{n \in \mathbb{Z}} u^{(n)} e^{i\alpha_n x}, \quad u^{(n)} = \frac{1}{\Lambda} \int_0^\Lambda u(x) e^{-i\alpha_n x} dx, \quad \alpha_n = \alpha + n \left(\frac{2\pi}{\Lambda} \right).$$

We define a trace functional space $H^s(\Gamma)$ with the norm given by

$$\|u\|_{H^s(\Gamma)} = \left(\Lambda \sum_{n \in \mathbb{Z}} (1 + \alpha_n^2)^s |u^{(n)}|^2 \right)^{1/2}.$$

Let $H_{S,qp}^1(\Omega)^2$ and $H^s(\Gamma)^2$ be the Cartesian product spaces equipped with the corresponding 2-norms of $H_{S,qp}^1(\Omega)$ and $H^s(\Gamma)$, respectively. It is known that $H^{-s}(\Gamma)^2$ is the dual space of $H^s(\Gamma)^2$ with respect to the $L^2(\Gamma)^2$ inner product

$$\langle \mathbf{u}, \mathbf{v} \rangle_\Gamma = \int_\Gamma \mathbf{u} \cdot \bar{\mathbf{v}} dx,$$

where the bar denotes the complex conjugate.

2.2. Boundary value problem. We wish to reduce the problem equivalently into a boundary value problem in Ω by introducing an exact transparent boundary condition on Γ .

The total field \mathbf{u} consists of the incident field \mathbf{u}_{inc} and the diffracted field \mathbf{v} , i.e.,

$$\mathbf{u} = \mathbf{u}_{\text{inc}} + \mathbf{v}. \quad (2.5)$$

Noting (2.5) and subtracting (2.4) from (2.1), we obtain the Navier equation for the diffracted field \mathbf{v} :

$$\mu \Delta \mathbf{v} + (\lambda + \mu) \nabla \nabla \cdot \mathbf{v} + \omega^2 \mathbf{v} = 0 \quad \text{in } \Omega^e. \quad (2.6)$$

For any solution \mathbf{v} of (2.6), we introduce the Helmholtz decomposition to split it into the compressional and shear parts:

$$\mathbf{v} = \nabla \phi_1 + \mathbf{curl} \phi_2, \quad (2.7)$$

where ϕ_1 and ϕ_2 are scalar potential functions. Substituting (2.7) into (2.6) gives

$$\nabla \left((\lambda + 2\mu) \Delta \phi_1 + \omega^2 \phi_1 \right) + \mathbf{curl} (\mu \Delta \phi_2 + \omega^2 \phi_2) = 0,$$

which is fulfilled if ϕ_j satisfy the Helmholtz equation

$$\Delta \phi_j + \kappa_j^2 \phi_j = 0, \quad (2.8)$$

where κ_j is the wavenumber defined in (2.3).

Since \mathbf{v} is a quasi-periodic function, we have from (2.7) that ϕ_j is also a quasi-periodic function in the x direction with period Λ and it has the Fourier series expansion

$$\phi_j(x, y) = \sum_{n \in \mathbb{Z}} \phi_j^{(n)}(y) e^{i\alpha_n x}. \quad (2.9)$$

Plugging (2.9) into (2.8) yields

$$\frac{d^2 \phi_j^{(n)}(y)}{dy^2} + (\beta_j^{(n)})^2 \phi_j^{(n)}(y) = 0, \quad y > b, \quad (2.10)$$

where

$$\beta_j^{(n)} = \begin{cases} (\kappa_j^2 - \alpha_n^2)^{1/2}, & |\alpha_n| < \kappa_j, \\ i(\alpha_n^2 - \kappa_j^2)^{1/2}, & |\alpha_n| > \kappa_j. \end{cases} \quad (2.11)$$

Note that $\beta_1^{(0)} = \beta = \kappa_1 \cos \theta$. We assume that $\kappa_j \neq |\alpha_n|$ for all $n \in \mathbb{Z}$ to exclude possible resonance. Noting (2.11) and using the bounded outgoing radiation condition, we obtain the solution of (2.10):

$$\phi_j^{(n)}(y) = \phi_j^{(n)}(b) e^{i\beta_j^{(n)}(y-b)},$$

which gives Rayleigh's expansion for ϕ_j :

$$\phi_j(x, y) = \sum_{n \in \mathbb{Z}} \phi_j^{(n)}(b) e^{i(\alpha_n x + \beta_j^{(n)}(y-b))}, \quad y > b. \quad (2.12)$$

Combining (2.12) and the Helmholtz decomposition (2.7) yields

$$\mathbf{v}(x, y) = i \sum_{n \in \mathbb{Z}} \begin{bmatrix} \alpha_n \\ \beta_1^{(n)} \end{bmatrix} \phi_1^{(n)}(b) e^{i(\alpha_n x + \beta_1^{(n)}(y-b))} + \begin{bmatrix} \beta_2^{(n)} \\ -\alpha_n \end{bmatrix} \phi_2^{(n)}(b) e^{i(\alpha_n x + \beta_2^{(n)}(y-b))}. \quad (2.13)$$

On the other hand, as a quasi-periodic function, the diffracted field \mathbf{v} also has the Fourier series expansion

$$\mathbf{v}(x, b) = \sum_{n \in \mathbb{Z}} \mathbf{v}^{(n)}(b) e^{i\alpha_n x}. \quad (2.14)$$

From (2.14) and (2.13), we obtain a linear system of algebraic equations for $\phi_j^{(n)}(b)$:

$$\begin{bmatrix} i\alpha_n & i\beta_2^{(n)} \\ i\beta_1^{(n)} & -i\alpha_n \end{bmatrix} \begin{bmatrix} \phi_1^{(n)}(b) \\ \phi_2^{(n)}(b) \end{bmatrix} = \begin{bmatrix} v_1^{(n)}(b) \\ v_2^{(n)}(b) \end{bmatrix}.$$

Solving the above equations via Cramer's rule gives

$$\phi_1^{(n)}(b) = -\frac{i}{\chi^{(n)}} (\alpha_n v_1^{(n)}(b) + \beta_2^{(n)} v_2^{(n)}(b)), \quad (2.15a)$$

$$\phi_2^{(n)}(b) = -\frac{i}{\chi^{(n)}} (\beta_1^{(n)} v_1^{(n)}(b) - \alpha_n v_2^{(n)}(b)), \quad (2.15b)$$

where

$$\chi^{(n)} = \alpha_n^2 + \beta_1^{(n)} \beta_2^{(n)}. \quad (2.16)$$

Plugging (2.15) into (2.13), we obtain Rayleigh's expansion for the diffracted field \mathbf{v} in Ω^e :

$$\begin{aligned} \mathbf{v}(x, y) = \sum_{n \in \mathbb{Z}} \frac{1}{\chi^{(n)}} & \begin{bmatrix} \alpha_n^2 & \alpha_n \beta_2^{(n)} \\ \alpha_n \beta_1^{(n)} & \beta_1^{(n)} \beta_2^{(n)} \end{bmatrix} \mathbf{v}^{(n)}(b) e^{i(\alpha_n x + \beta_1^{(n)}(y-b))} \\ & + \frac{1}{\chi^{(n)}} \begin{bmatrix} \beta_1^{(n)} \beta_2^{(n)} & -\alpha_n \beta_2^{(n)} \\ -\alpha_n \beta_1^{(n)} & \alpha_n^2 \end{bmatrix} \mathbf{v}^{(n)}(b) e^{i(\alpha_n x + \beta_2^{(n)}(y-b))}. \end{aligned} \quad (2.17)$$

Given a vector field $\mathbf{v} = [v_1, v_2]^\top$, we define a differential operator on Γ :

$$\mathcal{D}\mathbf{v} = \mu \partial_y \mathbf{v} + (\lambda + \mu) [0, 1]^\top \nabla \cdot \mathbf{v} = [\mu \partial_y v_1, (\lambda + \mu) \partial_x v_1 + (\lambda + 2\mu) \partial_y v_2]^\top. \quad (2.18)$$

By (2.18), and (2.17), we deduce the transparent boundary condition

$$\mathcal{D}\mathbf{v} = \mathcal{T}\mathbf{v} := \sum_{n \in \mathbb{Z}} M^{(n)} \mathbf{v}^{(n)}(b) e^{i\alpha_n x} \quad \text{on } \Gamma,$$

where the matrix

$$M^{(n)} = \frac{i}{\chi^{(n)}} \begin{bmatrix} \omega^2 \beta_1^{(n)} & \mu \alpha_n \chi^{(n)} - \omega^2 \alpha_n \\ \omega^2 \alpha_n - \mu \alpha_n \chi^{(n)} & \omega^2 \beta_2^{(n)} \end{bmatrix}.$$

Equivalently, we have the transparent boundary condition for the total field \mathbf{u} :

$$\mathcal{D}\mathbf{u} = \mathcal{T}\mathbf{u} + \mathbf{f} \quad \text{on } \Gamma,$$

where $\mathbf{f} = \mathcal{D}\mathbf{u}_{\text{inc}} - \mathcal{T}\mathbf{u}_{\text{inc}}$.

The scattering problem can be reduced to the following boundary value problem:

$$\begin{cases} \mu \Delta \mathbf{u} + (\lambda + \mu) \nabla \nabla \cdot \mathbf{u} + \omega^2 \mathbf{u} = 0 & \text{in } \Omega, \\ \mathbf{u} = 0 & \text{on } S, \\ \mathcal{D}\mathbf{u} = \mathcal{T}\mathbf{u} + \mathbf{f} & \text{on } \Gamma. \end{cases} \quad (2.19)$$

The weak formulation of (2.19) reads as follows: Find $\mathbf{u} \in H_{S,\text{qp}}^1(\Omega)^2$ such that

$$a(\mathbf{u}, \mathbf{v}) = \langle \mathbf{f}, \mathbf{v} \rangle_\Gamma, \quad \forall \mathbf{v} \in H_{S,\text{qp}}^1(\Omega)^2, \quad (2.20)$$

where the sesquilinear form $a : H_{S,\text{qp}}^1(\Omega)^2 \times H_{S,\text{qp}}^1(\Omega)^2 \rightarrow \mathbb{C}$ is defined by

$$\begin{aligned} a(\mathbf{u}, \mathbf{v}) = & \mu \int_\Omega \nabla \mathbf{u} : \nabla \bar{\mathbf{v}} \, d\mathbf{x} + (\lambda + \mu) \int_\Omega (\nabla \cdot \mathbf{u})(\nabla \cdot \bar{\mathbf{v}}) \, d\mathbf{x} \\ & - \omega^2 \int_\Omega \mathbf{u} \cdot \bar{\mathbf{v}} \, d\mathbf{x} - \langle T\mathbf{u}, \mathbf{v} \rangle_\Gamma. \end{aligned} \quad (2.21)$$

Here $A : B = \text{tr}(AB^\top)$ is the Frobenius inner product of square matrices A and B .

The existence of a unique weak solution \mathbf{u} of (2.20) is discussed in [23]. In this paper, we assume that the variational problem (2.20) admits a unique solution. It follows from the general theory in [3] that there exists a constant $\gamma_1 > 0$ such that the following inf-sup condition holds

$$\sup_{0 \neq \mathbf{v} \in H_{S,\text{qp}}^1(\Omega)^2} \frac{|a(\mathbf{u}, \mathbf{v})|}{\|\mathbf{v}\|_{H^1(\Omega)^2}} \geq \gamma_1 \|\mathbf{u}\|_{H^1(\Omega)^2}, \quad \forall \mathbf{u} \in H_{S,\text{qp}}^1(\Omega)^2. \quad (2.22)$$

2.3. Energy distribution. We study the energy distribution for the propagating reflected wave modes of the displacement. The result will be used to verify the accuracy of our numerical method when the analytic solution is not available.

Denote by $\boldsymbol{\nu} = (\nu_1, \nu_2)^\top$ and $\boldsymbol{\tau} = (\tau_1, \tau_2)^\top$ the unit normal and tangential vectors on S , where $\tau_1 = \nu_2$ and $\tau_2 = -\nu_1$. Let $\Delta_j^{(n)} = |\kappa_j^2 - \alpha_n^2|^{1/2}$ and $U_j = \{n : |\alpha_n| < \kappa_j\}$. We point out that U_1 and U_2 are the collections of all the propagating modes for the compressional and shear waves, respectively. It is clear to note that $\beta_j^{(n)} = \Delta_j^{(n)}$ for $n \in U_j$ and $\beta_j^{(n)} = i\Delta_j^{(n)}$ for $n \notin U_j$.

Consider the Helmholtz decomposition for the total field:

$$\mathbf{u} = \nabla \varphi_1 + \text{curl} \varphi_2. \quad (2.23)$$

Substituting (2.23) into (2.1), we may verify that φ_j also satisfies the Helmholtz equation

$$\Delta \varphi_j + \kappa_j^2 \varphi_j = 0 \quad \text{in } \Omega \cup \Omega^e.$$

Using the boundary condition (2.2), we have

$$\partial_\nu \varphi_1 - \partial_\tau \varphi_2 = 0 \quad \text{and} \quad \partial_\nu \varphi_2 + \partial_\tau \varphi_1 = 0 \quad \text{on } S.$$

Correspondingly, we introduce the Helmholtz decomposition for the incident field:

$$\mathbf{u}_{\text{inc}} = \nabla \psi_1 + \text{curl} \psi_2,$$

which gives explicitly that

$$\psi_1 = -\frac{1}{\kappa_1^2} \nabla \cdot \mathbf{u}_{\text{inc}} = -\frac{i}{\kappa_1} e^{i(\alpha x - \beta y)}, \quad \psi_2 = \frac{1}{\kappa_2^2} \text{curl} \mathbf{u}_{\text{inc}} = 0.$$

Hence we have

$$\varphi_1 = \phi_1 + \psi_1, \quad \varphi_2 = \phi_2.$$

Using the Rayleigh expansions (2.12), we get

$$\varphi_1(x, y) = r_0 e^{i(\alpha x - \beta y)} + \sum_{n \in \mathbb{Z}} r_1^{(n)} e^{i(\alpha_n x + \beta_1^{(n)} y)}, \quad (2.24)$$

$$\varphi_2(x, y) = \sum_{n \in \mathbb{Z}} r_2^{(n)} e^{i(\alpha_n x + \beta_2^{(n)} y)}, \quad (2.25)$$

where

$$r_0 = -\frac{i}{\kappa_1}, \quad r_1^{(n)} = \phi_1^{(n)}(b) e^{-i\beta_1^{(n)} b}, \quad r_2^{(n)} = \phi_2^{(n)}(b) e^{-i\beta_2^{(n)} b}.$$

The grating efficiency is defined by

$$e_1^{(n)} = \frac{\beta_1^{(n)} |r_1^{(n)}|^2}{\beta |r_0|^2}, \quad e_2^{(n)} = \frac{\beta_2^{(n)} |r_2^{(n)}|^2}{\beta |r_0|^2}, \quad (2.26)$$

where $e_1^{(n)}$ and $e_2^{(n)}$ are the efficiency of the n -th order reflected modes for the compressional wave and the shear wave, respectively. We have the following conservation of energy.

Theorem 2.2. *The total energy is conserved, i.e.,*

$$\sum_{n \in U_1} e_1^{(n)} + \sum_{n \in U_2} e_2^{(n)} = 1.$$

Proof. Consider the following coupled problem:

$$\begin{cases} \Delta \varphi_j + \kappa_j^2 \varphi_j = 0 & \text{in } \Omega, \\ \partial_\nu \varphi_1 - \partial_\tau \varphi_2 = 0 & \text{on } S, \\ \partial_\nu \varphi_2 + \partial_\tau \varphi_1 = 0 & \text{on } S. \end{cases} \quad (2.27)$$

It is clear to note that $\bar{\varphi}_j$ also satisfies the problem (2.27) since the wavenumber κ_j is real. Using Green's theorem and quasi-periodicity of the solution, we have

$$\begin{aligned} 0 &= \int_{\Omega} (\bar{\varphi}_1 \Delta \varphi_1 - \varphi_1 \Delta \bar{\varphi}_1) d\mathbf{x} + (\bar{\varphi}_2 \Delta \varphi_2 - \varphi_2 \Delta \bar{\varphi}_2) d\mathbf{x} \\ &= \int_S (\bar{\varphi}_1 \partial_\nu \varphi_1 - \varphi_1 \partial_\nu \bar{\varphi}_1) ds + \int_S (\bar{\varphi}_2 \partial_\nu \varphi_2 - \varphi_2 \partial_\nu \bar{\varphi}_2) ds \\ &\quad + \int_\Gamma (\bar{\varphi}_1 \partial_y \varphi_1 - \varphi_1 \partial_y \bar{\varphi}_1) dx + \int_\Gamma (\bar{\varphi}_2 \partial_y \varphi_2 - \varphi_2 \partial_y \bar{\varphi}_2) dx. \end{aligned} \quad (2.28)$$

It follows from integration by parts and the boundary conditions on S in (2.27) that

$$\begin{aligned} \int_S \bar{\varphi}_1 \partial_\nu \varphi_1 ds &= \int_S \bar{\varphi}_1 \partial_\tau \varphi_2 ds = - \int_S \varphi_2 \partial_\tau \bar{\varphi}_1 ds = \int_S \varphi_2 \partial_\nu \bar{\varphi}_2 ds, \\ \int_S \bar{\varphi}_2 \partial_\nu \varphi_2 ds &= - \int_S \bar{\varphi}_2 \partial_\tau \varphi_1 ds = \int_S \varphi_1 \partial_\tau \bar{\varphi}_2 ds = \int_S \varphi_1 \partial_\nu \bar{\varphi}_1 ds, \end{aligned}$$

which yields after taking the imaginary part of (2.28) that

$$\text{Im} \int_\Gamma (\bar{\varphi}_1 \partial_y \varphi_1 + \bar{\varphi}_2 \partial_y \varphi_2) dx = 0. \quad (2.29)$$

It follows from (2.24) and (2.25) that we have

$$\begin{aligned} \varphi_1(x, b) &= r_0 e^{i(\alpha x - \beta b)} + \sum_{n \in U_1} r_1^{(n)} e^{i(\alpha_n x + i\Delta_1^{(n)} b)} + \sum_{n \notin U_1} r_1^{(n)} e^{i(\alpha_n x - \Delta_1^{(n)} b)}, \\ \varphi_2(x, b) &= \sum_{n \in U_2} r_2^{(n)} e^{i(\alpha_n x + i\Delta_2^{(n)} b)} + \sum_{n \notin U_2} r_2^{(n)} e^{i(\alpha_n x - \Delta_2^{(n)} b)}, \end{aligned}$$

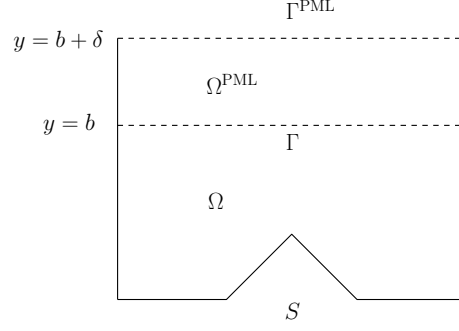


FIGURE 2. Geometry of the PML problem.

and

$$\begin{aligned}\partial_y \varphi_1(x, b) &= -i\beta r_0 e^{i(\alpha x - \beta b)} + \sum_{n \in U_1} i\Delta_1^{(n)} r_1^{(n)} e^{(i\alpha_n x + i\Delta_1^{(n)} b)} - \sum_{n \notin U_1} \Delta_1^{(n)} r_1^{(n)} e^{(i\alpha_n x - \Delta_1^{(n)} b)}, \\ \partial_y \varphi_2(x, b) &= \sum_{n \in U_2} i\Delta_2^{(n)} r_2^{(n)} e^{(i\alpha_n x + i\Delta_2^{(n)} b)} - \sum_{n \notin U_2} \Delta_2^{(n)} r_2^{(n)} e^{(i\alpha_n x - \Delta_2^{(n)} b)}.\end{aligned}$$

Substituting the above four functions into (2.29) and using the orthogonality of Fourier series, we get

$$\sum_{n \in U_1} \Delta_1^{(n)} |r_1^{(n)}|^2 + \sum_{n \in U_2} \Delta_2^{(n)} |r_2^{(n)}|^2 = \beta |r_0|^2,$$

which completes the proof. \square

In practice, the grating efficiencies (2.26) can be computed from (2.15) once the scattering problem is solved and the diffracted field \mathbf{v} is available on Γ .

3. THE PML PROBLEM

In this section, we shall introduce the PML formulation for the scattering problem and establish the well-posedness of the PML problem. An error estimate will be shown for the solutions between the original scattering problem and the PML problem.

3.1. PML formulation. Now we turn to the introduction of an absorbing PML layer. As is shown in Figure 2, the domain Ω is covered by a chunk of PML layer of thickness δ in Ω^e . Let $\rho(\tau) = \rho_1(\tau) + i\rho_2(\tau)$ be the PML function which is continuous and satisfies

$$\rho_1 = 1, \quad \rho_2 = 0 \quad \text{for } \tau < b \quad \text{and} \quad \rho_1 \geq 1, \quad \rho_2 > 0 \quad \text{otherwise.}$$

We introduce the PML by complex coordinate stretching:

$$\hat{y} = \int_0^y \rho(\tau) d\tau. \quad (3.1)$$

Let $\hat{\mathbf{x}} = (x, \hat{y})$. Introduce the new field

$$\hat{\mathbf{u}}(\mathbf{x}) = \begin{cases} \mathbf{u}_{\text{inc}}(\mathbf{x}) + (\mathbf{u}(\hat{\mathbf{x}}) - \mathbf{u}_{\text{inc}}(\hat{\mathbf{x}})), & \mathbf{x} \in \Omega^e, \\ \mathbf{u}(\hat{\mathbf{x}}), & \mathbf{x} \in \Omega. \end{cases} \quad (3.2)$$

It is clear to note that $\hat{\mathbf{u}}(\mathbf{x}) = \mathbf{u}(\mathbf{x})$ in Ω since $\hat{\mathbf{x}} = \mathbf{x}$ in Ω . It can be verified from (2.1) and (3.1) that $\hat{\mathbf{u}}$ satisfies

$$\mathcal{L}(\hat{\mathbf{u}} - \mathbf{u}_{\text{inc}}) = 0 \quad \text{in } \Omega \cup \Omega^e.$$

Here the PML differential operator

$$\mathcal{L}\mathbf{u} := \begin{bmatrix} (\lambda + 2\mu)\partial_x(\rho(y)\partial_x u_1) + \mu\partial_y(\rho^{-1}(y)\partial_y u_1) + (\lambda + \mu)\partial_{xy}^2 u_2 + \omega^2\rho(y)u_1 \\ \mu\partial_x(\rho(y)\partial_x u_2) + (\lambda + 2\mu)\partial_y(\rho^{-1}(y)\partial_y u_2) + (\lambda + \mu)\partial_{xy}^2 u_1 + \omega^2\rho(y)u_2 \end{bmatrix}.$$

Define the PML region

$$\Omega^{\text{PML}} = \{\mathbf{x} \in \mathbb{R}^2 : 0 < x < \Lambda, b < y < b + \delta\}.$$

Clearly, we have from (3.2) and (2.17) that the outgoing wave $\hat{\mathbf{u}}(\mathbf{x}) - \mathbf{u}_{\text{inc}}(\mathbf{x})$ in Ω^e decays exponentially as $y \rightarrow \infty$. Therefore, the homogeneous Dirichlet boundary condition can be imposed on

$$\Gamma^{\text{PML}} = \{\mathbf{x} \in \mathbb{R}^2 : 0 < x < \Lambda, y = b + \delta\}$$

to truncate the PML problem. Define the computational domain for the PML problem $D = \Omega \cup \Omega^{\text{PML}}$. We arrive at the following truncated PML problem: Find a quasi-periodic solution $\hat{\mathbf{u}}$ such that

$$\begin{cases} \mathcal{L}\hat{\mathbf{u}} = \mathbf{g} & \text{in } D, \\ \hat{\mathbf{u}} = \mathbf{u}_{\text{inc}} & \text{on } \Gamma^{\text{PML}}, \\ \hat{\mathbf{u}} = 0 & \text{on } S, \end{cases} \quad (3.3)$$

where

$$\mathbf{g} = \begin{cases} \mathcal{L}\mathbf{u}_{\text{inc}} & \text{in } \Omega^{\text{PML}}, \\ 0 & \text{in } \Omega. \end{cases}$$

Define $H_{0,\text{qp}}^1(D) = \{u \in H_{\text{qp}}^1(D) : u = 0 \text{ on } S \cup \Gamma^{\text{PML}}\}$. The weak formulation of the PML problem (3.3) reads as follows: Find $\hat{\mathbf{u}} \in H_{S,\text{qp}}^1(D)^2$ such that $\hat{\mathbf{u}} = \mathbf{u}_{\text{inc}}$ on Γ^{PML} and

$$b_D(\hat{\mathbf{u}}, \mathbf{v}) = - \int_D \mathbf{g} \cdot \bar{\mathbf{v}} d\mathbf{x}, \quad \forall \mathbf{v} \in H_{0,\text{qp}}^1(D)^2. \quad (3.4)$$

Here for any domain $G \subset \mathbb{R}^2$, the sesquilinear form $b_G : H_{\text{qp}}^1(G)^2 \times H_{\text{qp}}^1(G)^2 \rightarrow \mathbb{C}$ is defined by

$$\begin{aligned} b_G(\mathbf{u}, \mathbf{v}) = \int_G & (\lambda + 2\mu)(\rho\partial_x u_1 \partial_x \bar{v}_1 + \rho^{-1}\partial_y u_2 \partial_y \bar{v}_2) + \mu(\rho^{-1}\partial_y u_1 \partial_y \bar{v}_1 + \rho\partial_x u_2 \partial_x \bar{v}_2) \\ & + (\lambda + \mu)(\partial_x u_2 \partial_y \bar{v}_1 + \partial_x u_1 \partial_y \bar{v}_2) - \omega^2\rho(u_1 \bar{v}_1 + u_2 \bar{v}_2) d\mathbf{x}. \end{aligned}$$

We will reformulate the variational problem (3.4) in the domain D into an equivalent variational formulation in the domain Ω , and discuss the existence and uniqueness of the weak solution to the equivalent weak formulation. To do so, we need to introduce the transparent boundary condition for the truncated PML problem.

3.2. Transparent boundary condition of the PML problem. Let $\hat{\mathbf{v}}(\mathbf{x}) = \mathbf{v}(\hat{\mathbf{x}}) = \mathbf{u}(\hat{\mathbf{x}}) - \mathbf{u}_{\text{inc}}(\hat{\mathbf{x}})$. It is clear to note that $\hat{\mathbf{v}}$ satisfies the Navier equation in the complex coordinate

$$\mu\Delta_{\hat{\mathbf{x}}}\hat{\mathbf{v}} + (\lambda + \mu)\nabla_{\hat{\mathbf{x}}}\nabla_{\hat{\mathbf{x}}} \cdot \hat{\mathbf{v}} + \omega^2\hat{\mathbf{v}} = 0 \quad \text{in } \Omega^{\text{PML}}, \quad (3.5)$$

where $\nabla_{\hat{\mathbf{x}}} = [\partial_x, \partial_{\hat{y}}]^\top$ with $\partial_{\hat{y}} = \rho^{-1}(y)\partial_y$.

We introduce the Helmholtz decomposition to the solution of (3.5):

$$\hat{\mathbf{v}} = \nabla_{\hat{\mathbf{x}}}\hat{\phi}_1 + \text{curl}_{\hat{\mathbf{x}}}\hat{\phi}_2, \quad (3.6)$$

where $\text{curl}_{\hat{\mathbf{x}}} = [\partial_{\hat{y}}, -\partial_x]^\top$ and $\hat{\phi}_j(\mathbf{x}) = \phi_j(\hat{\mathbf{x}})$ satisfies the Helmholtz equation

$$\Delta_{\hat{\mathbf{x}}}\hat{\phi}_j + \kappa_j^2\hat{\phi}_j = 0. \quad (3.7)$$

Due to the quasi-periodicity of the solution, we have the Fourier series expansion

$$\hat{\phi}_j(x, y) = \sum_{n \in \mathbb{Z}} \hat{\phi}_j^{(n)}(y) e^{i\alpha_n x}. \quad (3.8)$$

Substituting (3.8) into (3.7) yields

$$\rho^{-1} \frac{d}{dy} \left(\rho^{-1} \frac{d}{dy} \hat{\phi}_j^{(n)}(y) \right) + (\beta_j^{(n)})^2 \hat{\phi}_j^{(n)}(y) = 0. \quad (3.9)$$

The general solutions of (3.9) is

$$\hat{\phi}_j^{(n)}(y) = A_j^{(n)} e^{i\beta_j^{(n)} \int_b^y \rho(\tau) d\tau} + B_j^{(n)} e^{-i\beta_j^{(n)} \int_b^y \rho(\tau) d\tau}.$$

Denote by

$$\zeta = \int_b^{b+\delta} \rho(\tau) d\tau. \quad (3.10)$$

The coefficients $A_j^{(n)}$ and $B_j^{(n)}$ can be uniquely determined by solving the following linear equations

$$\begin{bmatrix} \alpha_n & \alpha_n & \beta_2^{(n)} & -\beta_2^{(n)} \\ \beta_1^{(n)} & -\beta_1^{(n)} & -\alpha_n & -\alpha_n \\ \alpha_n e^{i\beta_1^{(n)} \zeta} & \alpha_n e^{-i\beta_1^{(n)} \zeta} & \beta_2^{(n)} e^{i\beta_2^{(n)} \zeta} & -\beta_2^{(n)} e^{-i\beta_2^{(n)} \zeta} \\ \beta_1^{(n)} e^{i\beta_1^{(n)} \zeta} & -\beta_1^{(n)} e^{-i\beta_1^{(n)} \zeta} & -\alpha_n e^{i\beta_2^{(n)} \zeta} & -\alpha_n e^{-i\beta_2^{(n)} \zeta} \end{bmatrix} \begin{bmatrix} A_1^{(n)} \\ B_1^{(n)} \\ A_2^{(n)} \\ B_2^{(n)} \end{bmatrix} = \begin{bmatrix} -i\hat{v}_1^{(n)}(b) \\ -i\hat{v}_2^{(n)}(b) \\ 0 \\ 0 \end{bmatrix}, \quad (3.11)$$

where we have used the Helmholtz decomposition (3.6) and the homogeneous Dirichlet boundary condition

$$\hat{v}(x, b + \delta) = 0 \quad \text{on } \Gamma^{\text{PML}}$$

due to the PML absorbing layer. Solving the linear equations (3.11), we obtain

$$\begin{aligned} A_1^{(n)} &= \frac{i}{2\chi^{(n)} \hat{\chi}^{(n)}} \left\{ -\chi^{(n)} (\varepsilon_1^{(n)} + 2) (\alpha_n \hat{v}_1^{(n)}(b) + \beta_2^{(n)} \hat{v}_2^{(n)}(b)) \right. \\ &\quad \left. + 2\beta_2^{(n)} (\varepsilon_1^{(n)} + 2\delta_1^{(n)}) (1 + \delta_2^{(n)} - \eta^{(n)}) (\alpha_n \beta_1^{(n)} \hat{v}_1^{(n)}(b) + \alpha_n^2 \hat{v}_2^{(n)}(b)) \right\}, \\ B_1^{(n)} &= \frac{i}{2\chi^{(n)} \hat{\chi}^{(n)}} \left\{ \chi^{(n)} \varepsilon_1^{(n)} (\alpha_n \hat{v}_1^{(n)}(b) - \beta_2^{(n)} \hat{v}_2^{(n)}(b)) \right. \\ &\quad \left. + 2(\varepsilon_1^{(n)} \delta_2^{(n)} + 2(\delta_1^{(n)} + \delta_1^{(n)} \delta_2^{(n)})) (\alpha_n \beta_1^{(n)} \beta_2^{(n)} \hat{v}_1^{(n)}(b) - \alpha_n^2 \beta_2^{(n)} \hat{v}_2^{(n)}(b)) \right\}, \\ A_2^{(n)} &= \frac{i}{2\chi^{(n)} \hat{\chi}^{(n)}} \left\{ \chi^{(n)} [\varepsilon_1^{(n)} \eta^{(n)} - 2(\varepsilon_1^{(n)} + 1)(1 + \delta_2^{(n)})] (\beta_1^{(n)} \hat{v}_1^{(n)}(b) - \alpha_n \hat{v}_2^{(n)}(b)) \right. \\ &\quad \left. + 2\varepsilon_1^{(n)} (1 + \delta_2^{(n)} - \eta^{(n)}) ((\beta_1^{(n)})^2 \beta_2^{(n)} \hat{v}_1^{(n)}(b) - \alpha_n^3 \hat{v}_2^{(n)}(b)) \right\}, \\ B_2^{(n)} &= \frac{i}{2\chi^{(n)} \hat{\chi}^{(n)}} \left\{ \chi^{(n)} [2\delta_2^{(n)} (\varepsilon_1^{(n)} + 1) - \varepsilon_1^{(n)} \eta^{(n)}] (\beta_1^{(n)} \hat{v}_1^{(n)}(b) + \alpha_n \hat{v}_2^{(n)}(b)) \right. \\ &\quad \left. - 2\delta_2^{(n)} (\varepsilon_1^{(n)} + 2) ((\beta_1^{(n)})^2 \beta_2^{(n)} \hat{v}_1^{(n)}(b) + \alpha_n^3 \hat{v}_2^{(n)}(b)) \right\}, \end{aligned}$$

where

$$\begin{cases} \varepsilon_j^{(n)} &= \coth(-i\beta_j^{(n)} \zeta) - 1, \\ \delta_j^{(n)} &= (e^{i\beta_2^{(n)} \zeta} - e^{i\beta_1^{(n)} \zeta}) / (e^{-i\beta_j^{(n)} \zeta} - e^{i\beta_j^{(n)} \zeta}), \\ \eta^{(n)} &= \delta_2^{(n)} / \delta_1^{(n)} = (e^{-i\beta_1^{(n)} \zeta} - e^{i\beta_1^{(n)} \zeta}) / (e^{-i\beta_2^{(n)} \zeta} - e^{i\beta_2^{(n)} \zeta}) \end{cases} \quad (3.12)$$

and

$$\hat{\chi}^{(n)} = \chi^{(n)} + 4(\delta_2^{(n)} - \delta_1^{(n)} - \delta_1^{(n)} \delta_2^{(n)}) \alpha_n^2 \beta_1^{(n)} \beta_2^{(n)} / \chi^{(n)}. \quad (3.13)$$

Here, the hyperbolic cotangent function is defined as

$$\coth(t) = (e^t + e^{-t}) / (e^t - e^{-t}).$$

Following the Helmholtz decomposition (3.6) again, we have

$$\begin{aligned} \hat{\mathbf{v}}(x, y) = i \sum_{n \in \mathbb{Z}} \begin{bmatrix} \alpha_n \\ \beta_1^{(n)} \end{bmatrix} A_1^{(n)} e^{i(\alpha_n x + \beta_1^{(n)} \int_b^y \rho(\tau) d\tau)} + \begin{bmatrix} \alpha_n \\ -\beta_1^{(n)} \end{bmatrix} B_1^{(n)} e^{i(\alpha_n x - \beta_1^{(n)} \int_b^y \rho(\tau) d\tau)} \\ \begin{bmatrix} \beta_2^{(n)} \\ -\alpha_n \end{bmatrix} A_2^{(n)} e^{i(\alpha_n x + \beta_2^{(n)} \int_b^y \rho(\tau) d\tau)} - \begin{bmatrix} \beta_2^{(n)} \\ \alpha_n \end{bmatrix} B_2^{(n)} e^{i(\alpha_n x - \beta_2^{(n)} \int_b^y \rho(\tau) d\tau)}. \end{aligned} \quad (3.14)$$

Combining (3.14) and (2.18), we derive the transparent boundary condition for the PML problem on Γ :

$$\mathcal{D}\hat{\mathbf{v}} = \mathcal{T}^{\text{PML}}\hat{\mathbf{v}} := \sum_{n \in \mathbb{Z}} \hat{M}^{(n)} \hat{\mathbf{v}}^{(n)}(b) e^{i\alpha_n x},$$

where the matrix

$$\hat{M}^{(n)} = \begin{bmatrix} \hat{m}_{11}^{(n)} & \hat{m}_{12}^{(n)} \\ \hat{m}_{21}^{(n)} & \hat{m}_{22}^{(n)} \end{bmatrix}.$$

Here the entries are

$$\begin{aligned} \hat{m}_{11}^{(n)} &= \frac{i\omega^2 \beta_1^{(n)}}{\hat{\chi}^{(n)}} + \frac{i\omega^2 \beta_1^{(n)}}{\chi^{(n)} \hat{\chi}^{(n)}} \left[\varepsilon_1^{(n)} \alpha_n^2 + (\varepsilon_1^{(n)} \eta^{(n)} + 2\delta_2^{(n)}) \beta_1^{(n)} \beta_2^{(n)} \right], \\ \hat{m}_{12}^{(n)} &= i\mu \alpha_n - \frac{i\omega^2 \alpha_n}{\hat{\chi}^{(n)}} - \frac{i\omega^2 \alpha_n \beta_1^{(n)} \beta_2^{(n)}}{\chi^{(n)} \hat{\chi}^{(n)}} \left[\varepsilon_1^{(n)} (1 + 2\delta_2^{(n)} - \eta^{(n)}) + 2\delta_2^{(n)} \right], \\ \hat{m}_{21}^{(n)} &= -i\mu \alpha_n + \frac{i\omega^2 \alpha_n}{\hat{\chi}^{(n)}} - \frac{i\omega^2 \alpha_n \beta_1^{(n)} \beta_2^{(n)}}{\chi^{(n)} \hat{\chi}^{(n)}} \left[\varepsilon_1^{(n)} (1 + 2\delta_2^{(n)} - \eta^{(n)}) + 2(2\delta_1^{(n)} + 2\delta_1^{(n)} \delta_2^{(n)} - \delta_2^{(n)}) \right], \\ \hat{m}_{22}^{(n)} &= \frac{i\omega^2 \beta_2^{(n)}}{\hat{\chi}^{(n)}} + \frac{i\omega^2 \beta_2^{(n)}}{\chi^{(n)} \hat{\chi}^{(n)}} \left[\varepsilon_1^{(n)} \beta_1^{(n)} \beta_2^{(n)} + (\varepsilon_1^{(n)} \eta^{(n)} + 2\delta_2^{(n)}) \alpha_n^2 \right]. \end{aligned}$$

Equivalently, we have the transparent boundary condition for the total field $\hat{\mathbf{u}}$ on Γ :

$$\mathcal{D}\hat{\mathbf{u}} = \mathcal{T}^{\text{PML}}\hat{\mathbf{u}} + \mathbf{f}^{\text{PML}},$$

where $\mathbf{f}^{\text{PML}} = \mathcal{D}\hat{\mathbf{u}}_{\text{inc}} - \mathcal{T}^{\text{PML}}\hat{\mathbf{u}}_{\text{inc}}$.

The PML problem can be reduced to the following boundary value problem:

$$\begin{cases} \mu \Delta \mathbf{u}^{\text{PML}} + (\lambda + \mu) \nabla \nabla \cdot \mathbf{u}^{\text{PML}} + \omega^2 \mathbf{u}^{\text{PML}} = 0 & \text{in } \Omega, \\ \mathbf{u}^{\text{PML}} = 0 & \text{on } S, \\ \mathcal{D}\mathbf{u}^{\text{PML}} = \mathcal{T}^{\text{PML}}\mathbf{u}^{\text{PML}} + \mathbf{f}^{\text{PML}} & \text{on } \Gamma. \end{cases} \quad (3.15)$$

The weak formulation of (3.15) is to find $\mathbf{u}^{\text{PML}} \in H_{S, \text{qp}}^1(\Omega)^2$ such that

$$a^{\text{PML}}(\mathbf{u}^{\text{PML}}, \mathbf{v}) = \langle \mathbf{f}^{\text{PML}}, \mathbf{v} \rangle_{\Gamma}, \quad \forall \mathbf{v} \in H_{S, \text{qp}}^1(\Omega)^2, \quad (3.16)$$

where the sesquilinear form $a^{\text{PML}} : H_{S, \text{qp}}^1(\Omega)^2 \times H_{S, \text{qp}}^1(\Omega)^2 \rightarrow \mathbb{C}$ is defined by

$$\begin{aligned} a^{\text{PML}}(\mathbf{u}, \mathbf{v}) &= \mu \int_{\Omega} \nabla \mathbf{u} : \nabla \bar{\mathbf{v}} d\mathbf{x} + (\lambda + \mu) \int_{\Omega} (\nabla \cdot \mathbf{u})(\nabla \cdot \bar{\mathbf{v}}) d\mathbf{x} \\ &\quad - \omega^2 \int_{\Omega} \mathbf{u} \cdot \bar{\mathbf{v}} d\mathbf{x} - \langle \mathcal{T}^{\text{PML}}\mathbf{u}, \mathbf{v} \rangle_{\Gamma}. \end{aligned} \quad (3.17)$$

The following lemma establishes the relationship between the variational problem (3.16) and the weak formulation (3.4). The proof is straightforward based on our constructions of the transparent boundary conditions for the PML problem. The details of the proof is omitted for brevity.

Lemma 3.1. *Any solution $\hat{\mathbf{u}}$ of the variational problem (3.4) restricted to Ω is a solution of the variational (3.16); conversely, any solution \mathbf{u}^{PML} of the variational problem (3.16) can be uniquely extended to the whole domain to be a solution $\hat{\mathbf{u}}$ of the variational problem (3.4) in D .*

3.3. Convergence of the PML solution. Now we turn to estimating the error between \mathbf{u}^{PML} and \mathbf{u} . The key is to estimate the error of the boundary operators \mathcal{T}^{PML} and \mathcal{T} .

Let

$$\Delta_j^- = \min\{\Delta_j^{(n)} : n \in U_j\}, \quad \Delta_j^+ = \min\{\Delta_j^{(n)} : n \notin U_j\}.$$

Denote

$$F = \max_{j=1,2} \left(\frac{\Delta_j^-}{e^{\frac{1}{2}\Delta_j^- \text{Im}\zeta} - 1}, \frac{\Delta_j^+}{e^{\frac{1}{2}\Delta_j^+ \text{Re}\zeta} - 1} \right) \\ \times \max \left\{ 12\kappa_2, 16\kappa_2^4, 8 + 2\kappa_2^2, \frac{16\kappa_2^3}{\kappa_1^2}, \frac{24(16 + \kappa_2^2)^2}{\kappa_1^2} \right\}.$$

The constant F will be used to control the modeling error between the PML problem and the original scattering problem. Once the incoming plane wave \mathbf{u}_{inc} is fixed, the quantities Δ_j^-, Δ_j^+ are fixed. Thus the constant F approaches to zero exponentially as the PML parameters $\text{Re}\zeta$ and $\text{Im}\zeta$ tend to infinity. Recalling the definition of ζ in (3.10), we know that $\text{Re}\zeta$ and $\text{Im}\zeta$ can be calculated by the medium property $\rho(y)$, which is usually taken as a power function:

$$\rho(y) = 1 + \sigma \left(\frac{y-b}{\delta} \right)^m \quad \text{if } y \geq b, \quad m \geq 1.$$

Thus we have

$$\text{Re}\zeta = \left(1 + \frac{\text{Re}\sigma}{m+1} \right) \delta, \quad \text{Im}\zeta = \left(\frac{\text{Im}\sigma}{m+1} \right) \delta.$$

In practice, we may pick some appropriate PML parameters σ and δ such that $\text{Re}\zeta \geq 1$.

Lemma 3.2. *For any $\mathbf{u}, \mathbf{v} \in H_{S,\text{qp}}^1(\Omega)^2$, we have*

$$|\langle (\mathcal{T}^{\text{PML}} - \mathcal{T})\mathbf{u}, \mathbf{v} \rangle_{\Gamma}| \leq \hat{F} \|\mathbf{u}\|_{L^2(\Gamma)^2} \|\mathbf{v}\|_{L^2(\Gamma)^2},$$

where $\hat{F} = 17\omega^2 F / \kappa_1^4$.

Proof. For any $\mathbf{u}, \mathbf{v} \in H_{S,\text{qp}}^1(\Omega)^2$, we have the following Fourier series expansions:

$$\mathbf{u}(x, b) = \sum_{n \in \mathbb{Z}} \mathbf{u}^{(n)}(b) e^{i\alpha_n x}, \quad \mathbf{v}(x, b) = \sum_{n \in \mathbb{Z}} \mathbf{v}^{(n)}(b) e^{i\alpha_n x},$$

which gives

$$\|\mathbf{u}\|_{L^2(\Gamma)^2}^2 = \Lambda \sum_{n \in \mathbb{Z}} |\mathbf{u}^{(n)}(b)|^2, \quad \|\mathbf{v}\|_{L^2(\Gamma)^2}^2 = \Lambda \sum_{n \in \mathbb{Z}} |\mathbf{v}^{(n)}(b)|^2.$$

It follows from the orthogonality of Fourier series, the Cauchy–Schwarz inequality, and Proposition A.4 that we have

$$|\langle (\mathcal{T}^{\text{PML}} - \mathcal{T})\mathbf{u}, \mathbf{v} \rangle_{\Gamma}| = \left| \Lambda \sum_{n \in \mathbb{Z}} ((M^{(n)} - \hat{M}^{(n)})\mathbf{u}^{(n)}(b)) \cdot \bar{\mathbf{v}}^{(n)}(b) \right| \\ \leq \left(\Lambda \sum_{n \in \mathbb{Z}} \|M^{(n)} - \hat{M}^{(n)}\|_2^2 |\mathbf{u}^{(n)}(b)|^2 \right)^{1/2} \left(\Lambda \sum_{n \in \mathbb{Z}} |\mathbf{v}^{(n)}(b)|^2 \right)^{1/2} \leq \hat{F} \|\mathbf{u}\|_{L^2(\Gamma)^2} \|\mathbf{v}\|_{L^2(\Gamma)^2},$$

which completes the proof. \square

Let $a = \min_y \{x \in S\}$. Denote $\tilde{\Omega} = \{x \in \mathbb{R}^2 : 0 < x < \Lambda, a < y < b\}$.

Lemma 3.3. *For any $\mathbf{u} \in H_{S,\text{qp}}^1(\Omega)^2$, we have*

$$\|\mathbf{u}\|_{L^2(\Gamma)^2} \leq \|\mathbf{u}\|_{H^{1/2}(\Gamma)^2} \leq \gamma_2 \|\mathbf{u}\|_{H^1(\Omega)^2},$$

where $\gamma_2 = (1 + (b-a)^{-1})^{1/2}$.

Proof. First we have

$$\begin{aligned} (b-a)|u(b)|^2 &= \int_a^b |u(y)|^2 dy + \int_a^b \int_y^b \frac{d}{dt} |u(t)|^2 dt dy \\ &\leq \int_a^b |u(y)|^2 dy + (b-a) \int_a^b 2|u(y)||u'(y)| dy, \end{aligned}$$

which gives by applying the Cauchy–Schwarz inequality that

$$(1 + \alpha_n^2)^{1/2} |u(b)|^2 \leq \gamma_2^2 (1 + \alpha_n^2) \int_a^b |u(y)|^2 dy + \int_a^b |u'(y)|^2 dy.$$

Given $\mathbf{u} \in H_{S,\text{qp}}^1(\Omega)^2$, we consider the zero extension

$$\tilde{\mathbf{u}} = \begin{cases} \mathbf{u} & \text{in } \Omega, \\ 0 & \text{in } \tilde{\Omega} \setminus \bar{\Omega}, \end{cases}$$

which has the Fourier series expansion

$$\tilde{\mathbf{u}}(x, y) = \sum_{n \in \mathbb{Z}} \tilde{\mathbf{u}}^{(n)}(y) e^{i\alpha_n x} \quad \text{in } \tilde{\Omega}.$$

By definitions, we have

$$\|\tilde{\mathbf{u}}\|_{H^{1/2}(\Gamma)^2}^2 = \Lambda \sum_{n \in \mathbb{Z}} (1 + \alpha_n^2)^{1/2} |\tilde{\mathbf{u}}^{(n)}(b)|^2$$

and

$$\|\tilde{\mathbf{u}}\|_{H^1(\tilde{\Omega})^2}^2 = \Lambda \sum_{n \in \mathbb{Z}} \int_a^b (1 + \alpha_n^2) |\tilde{\mathbf{u}}^{(n)}(y)|^2 + |\mathbf{u}^{(n)'}(y)|^2 dy.$$

Noting $\|\mathbf{u}\|_{H^{1/2}(\Gamma)^2} = \|\tilde{\mathbf{u}}\|_{H^{1/2}(\Gamma)^2}$ and $\|\mathbf{u}\|_{H^1(\Omega)^2} = \|\tilde{\mathbf{u}}\|_{H^1(\tilde{\Omega})^2}$, we complete the proof by combining the above estimates. \square

Theorem 3.4. *Let γ_1 and γ_2 be the constants in the inf-sup condition (2.22) and in Lemma 3.3, respectively. If $\hat{F}\gamma_2^2 < \gamma_1$, then the PML variational problem (3.16) has a unique weak solution \mathbf{u}^{PML} , which satisfies the error estimate*

$$\|\mathbf{u} - \mathbf{u}^{\text{PML}}\|_{\Omega} := \sup_{0 \neq \mathbf{v} \in H_{S,\text{qp}}^1(\Omega)^2} \frac{|a(\mathbf{u} - \mathbf{u}^{\text{PML}}, \mathbf{v})|}{\|\mathbf{v}\|_{H^1(\Omega)^2}} \leq \hat{F}\gamma_2 \|\mathbf{u}^{\text{PML}} - \mathbf{u}_{\text{inc}}\|_{L^2(\Gamma)^2}, \quad (3.18)$$

where \mathbf{u} is the unique weak solution of the variational problem (2.20).

Proof. It suffices to show the coercivity of the sesquilinear form a^{PML} defined in (3.17) in order to prove the unique solvability of the weak problem (3.16). Using Lemmas 3.2, 3.3 and the assumption $\hat{F}\gamma_2^2 < \gamma_1$, we get for any \mathbf{u}, \mathbf{v} in $H_{S,\text{qp}}^1(\Omega)^2$ that

$$\begin{aligned} |a^{\text{PML}}(\mathbf{u}, \mathbf{v})| &\geq |a(\mathbf{u}, \mathbf{v})| - |\langle (\mathcal{T}^{\text{PML}} - \mathcal{T})\mathbf{u}, \mathbf{v} \rangle_{\Gamma}| \\ &\geq |a(\mathbf{u}, \mathbf{v})| - \hat{F}\gamma_2^2 \|\mathbf{u}\|_{H^1(\Omega)^2} \|\mathbf{v}\|_{H^1(\Omega)^2} \\ &\geq (\gamma_1 - \hat{F}\gamma_2^2) \|\mathbf{u}\|_{H^1(\Omega)^2} \|\mathbf{v}\|_{H^1(\Omega)^2}. \end{aligned}$$

It remains to show the error estimate (3.18). It follows from (2.20)–(2.21) and (3.16)–(3.17) that

$$\begin{aligned} a(\mathbf{u} - \mathbf{u}^{\text{PML}}, \mathbf{v}) &= a(\mathbf{u}, \mathbf{v}) - a(\mathbf{u}^{\text{PML}}, \mathbf{v}) \\ &= \langle \mathbf{f}, \mathbf{v} \rangle_{\Gamma} - \langle \mathbf{f}^{\text{PML}}, \mathbf{v} \rangle_{\Gamma} + a^{\text{PML}}(\mathbf{u}^{\text{PML}}, \mathbf{v}) - a(\mathbf{u}^{\text{PML}}, \mathbf{v}) \\ &= \langle (\mathcal{T}^{\text{PML}} - \mathcal{T})\mathbf{u}_{\text{inc}}, \mathbf{v} \rangle_{\Gamma} - \langle (\mathcal{T}^{\text{PML}} - \mathcal{T})\mathbf{u}^{\text{PML}}, \mathbf{v} \rangle_{\Gamma} \\ &= \langle (\mathcal{T} - \mathcal{T}^{\text{PML}})(\mathbf{u}^{\text{PML}} - \mathbf{u}_{\text{inc}}), \mathbf{v} \rangle_{\Gamma}, \end{aligned}$$

which completes the proof upon using Lemmas 3.2 and 3.3. \square

We remark that the error estimate (3.18) is a posteriori in nature as it depends only on the PML solution \mathbf{u}^{PML} , which makes a posteriori error control possible. Moreover, the PML approximation error can be reduced exponentially by either enlarging the thickness δ of the PML layers or enlarging the medium parameters $\text{Re}\sigma$ and $\text{Im}\sigma$.

4. FINITE ELEMENT APPROXIMATION

In this section, we consider the finite element approximation of the PML problem (3.4) and deduce the a posteriori error estimate.

4.1. The discrete problem. Let \mathcal{M}_h be a regular triangulation of the domain D . Every triangle $T \in \mathcal{M}_h$ is considered as closed. We assume that any element T must be completely included in $\overline{\Omega^{\text{PML}}}$ or $\overline{\Omega}$. In order to introduce a finite element space whose functions are quasi-periodic in the x direction, we require that if $(0, y)$ is a node on the left boundary, then (Λ, y) is also a node on the right boundary, and vice versa. Let $V_h(D) \subset H_{\text{qp}}^1(D)$ be a conforming finite element space, and $\dot{V}_h(D) = V_h(D) \cap H_{0,\text{qp}}^1(D)$.

Denote by $\Pi_h : C(\bar{D})^2 \rightarrow V_h(D)^2$ the Scott–Zhang interpolation operator, which has the following properties:

$$\|\mathbf{v} - \Pi_h \mathbf{v}\|_{L^2(T)^2} \leq Ch_T \|\nabla \mathbf{v}\|_{F(\tilde{T})}, \quad \|\mathbf{v} - \Pi_h \mathbf{v}\|_{L^2(e)^2} \leq Ch_e^{1/2} \|\nabla \mathbf{v}\|_{F(\tilde{e})},$$

where h_T is the diameter of the triangle T , h_e is the length of the edge e , \tilde{T} and \tilde{e} are the unions of all elements which have nonempty intersection with the element T and the edge e , respectively, and the Frobenius norm of the Jacobian matrix $\nabla \mathbf{v}$ is defined by

$$\|\nabla \mathbf{v}\|_{F(G)} = \left(\sum_{j=1}^2 \int_G |\nabla v_j|^2 dx \right)^{1/2}.$$

The finite element approximation to the problem (3.4) reads as follows: Find $\hat{\mathbf{u}}_h \in V_h(D)^2$ such that $\hat{\mathbf{u}}_h = \Pi_h \mathbf{u}_{\text{inc}}$ on Γ^{PML} , $\hat{\mathbf{u}}_h = 0$ on S , and

$$b_D(\hat{\mathbf{u}}_h, \mathbf{v}_h) = - \int_D \mathbf{g} \cdot \bar{\mathbf{v}}_h dx, \quad \forall \mathbf{v}_h \in \dot{V}_h(D)^2. \quad (4.1)$$

Following the general theory in [3], the existence of a unique solution of the discrete problem (4.1) and the finite element convergence analysis depend on the following discrete inf-sup condition:

$$\sup_{0 \neq \mathbf{v}_h \in \dot{V}_h(D)^2} \frac{|b(\hat{\mathbf{u}}_h, \mathbf{v}_h)|}{\|\mathbf{v}_h\|_{H^1(D)^2}} \geq \gamma_0 \|\hat{\mathbf{u}}_h\|_{H^1(D)^2}, \quad \forall \hat{\mathbf{u}}_h \in \dot{V}_h(D)^2, \quad (4.2)$$

where the constant $\gamma_0 > 0$ is independent of the finite element mesh size. Since the continuous problem (3.4) has a unique solution by Theorem 3.4, the sesquilinear form $b : H_{\text{qp}}^1(D)^2 \times H_{\text{qp}}^1(D)^2 \rightarrow \mathbb{C}$ satisfies the continuous inf-sup condition. Then a general argument of Schatz [30] implies that (4.2) is valid for sufficiently small mesh size $h < h^*$. Thanks to (4.2), an appropriate a priori error estimate can be derived and the estimate depends on the regularity of the PML solution \mathbf{u}^{PML} . We assume that the discrete problem (4.1) admits a unique solution $\hat{\mathbf{u}}_h \in V_h(D)^2$, since we are interested in the a posteriori error estimate and the associated adaptive algorithm.

Denote by \mathcal{B}_h the set of all sides that do not lie on Γ^{PML} and S . For any $T \in \mathcal{M}_h$, we introduce the residual

$$R_T := (\mathcal{L}\hat{\mathbf{u}}_h + \mathbf{g})|_T = \begin{cases} \mathcal{L}(\hat{\mathbf{u}}_h - \mathbf{u}_{\text{inc}})|_T & \text{if } T \in \Omega^{\text{PML}}, \\ \mathcal{L}\hat{\mathbf{u}}_h|_T & \text{otherwise.} \end{cases}$$

For any interior side $e \in \mathcal{B}_h$ which is the common side of T_1 and T_2 , we define the jump residual across e as

$$J_e = \mathcal{D}_\nu \hat{\mathbf{u}}_h|_{T_1} - \mathcal{D}_\nu \hat{\mathbf{u}}_h|_{T_2},$$

where the unit normal vector $\boldsymbol{\nu}$ on e points from T_2 to T_1 and the differential operator

$$\mathcal{D}_{\boldsymbol{\nu}} \mathbf{v} = \mu \partial_{\boldsymbol{\nu}} \mathbf{v} + (\lambda + \mu)(\nabla \cdot \mathbf{v}) \boldsymbol{\nu}.$$

Define

$$\Gamma_{\text{left}} = \{\mathbf{x} \in \partial D : x = 0\}, \quad \Gamma_{\text{right}} = \{\mathbf{x} \in \partial D : x = \Lambda\}.$$

If $e = \Gamma_{\text{left}} \cap \partial T$ for some element $T \in \mathcal{M}_h$ and e' be the corresponding side on Γ_{right} , which is also a side for some element T' , then we define the jump residual as

$$\begin{aligned} J_e &= \left[\mu \partial_x (\hat{\mathbf{u}}_h|_T) + (\lambda + \mu)[1, 0]^\top \nabla_{\hat{\mathbf{x}}} \cdot (\hat{\mathbf{u}}_h|_T) \right] - e^{-i\alpha\Lambda} \left[\mu \partial_x (\hat{\mathbf{u}}_h|_{T'}) + (\lambda + \mu)[1, 0]^\top \nabla_{\hat{\mathbf{x}}} \cdot (\hat{\mathbf{u}}_h|_{T'}) \right], \\ J_{e'} &= e^{i\alpha\Lambda} \left[\mu \partial_x (\hat{\mathbf{u}}_h|_T) + (\lambda + \mu)[1, 0]^\top \nabla_{\hat{\mathbf{x}}} \cdot (\hat{\mathbf{u}}_h|_T) \right] - \left[\mu \partial_x (\hat{\mathbf{u}}_h|_{T'}) + (\lambda + \mu)[1, 0]^\top \nabla_{\hat{\mathbf{x}}} \cdot (\hat{\mathbf{u}}_h|_{T'}) \right]. \end{aligned}$$

For any $T \in \mathcal{M}_h$, denote by η_T the local error estimator:

$$\eta_T = h_T \|R_T\|_{L^2(T)^2} + \left(\frac{1}{2} \sum_{e \subset \partial T} h_e \|J_e\|_{L^2(e)^2}^2 \right)^{1/2}.$$

The following theorem is the main result of this paper.

Theorem 4.1. *There exists a positive constant C such that the following a posteriori error estimate holds*

$$\begin{aligned} \|\mathbf{u} - \hat{\mathbf{u}}_h\|_{H^1(\Omega)^2} &\leq \gamma_2 \hat{F} \|\hat{\mathbf{u}}_h - \mathbf{u}_{\text{inc}}\|_{L^2(\Gamma)^2} + \gamma_2 C_2 \|\Pi_h \mathbf{u}_{\text{inc}} - \mathbf{u}_{\text{inc}}\|_{L^2(\Gamma^{\text{PML}})^2} \\ &\quad + C(1 + \gamma_2 C_1) \left(\sum_{T \in \mathcal{M}_h} \eta_T^2 \right)^{1/2}, \end{aligned}$$

where the constants \hat{F} , γ_2 , and C_j are defined in Lemmas 3.2, 3.3, 4.3, 4.4, respectively.

4.2. A posteriori error analysis. For any $\mathbf{v} \in H_{\text{qp}}^1(\Omega)^2$, we denote by $\tilde{\mathbf{v}}$ the extension of \mathbf{v} such that $\tilde{\mathbf{v}} = \mathbf{v}$ in Ω and $\tilde{\mathbf{v}}$ satisfies the following boundary value problem

$$\begin{cases} \mu \Delta_{\hat{\mathbf{x}}} \tilde{\mathbf{v}} + (\lambda + \mu) \nabla_{\hat{\mathbf{x}}} \nabla_{\hat{\mathbf{x}}} \cdot \tilde{\mathbf{v}} + \omega^2 \tilde{\mathbf{v}} = 0 & \text{in } \Omega^{\text{PML}}, \\ \tilde{\mathbf{v}}(x, b) = \mathbf{v}(x, b) & \text{on } \Gamma, \\ \tilde{\mathbf{v}}(x, b + \delta) = 0 & \text{on } \Gamma^{\text{PML}}. \end{cases} \quad (4.3)$$

Lemma 4.2. *For any $\mathbf{u}, \mathbf{v} \in H_{\text{qp}}^1(\Omega)^2$ we have*

$$\int_{\Gamma} \mathcal{T}^{\text{PML}} \mathbf{u} \cdot \tilde{\mathbf{v}} dx = \int_{\Gamma} \mathbf{u} \cdot \mathcal{D} \tilde{\mathbf{v}} dx.$$

Proof. Introduce a function $\hat{\mathbf{w}} \in H_{\text{qp}}^1(\Omega^{\text{PML}})^2$ which satisfies

$$\begin{cases} \mu \Delta_{\hat{\mathbf{x}}} \hat{\mathbf{w}} + (\lambda + \mu) \nabla_{\hat{\mathbf{x}}} \nabla_{\hat{\mathbf{x}}} \cdot \hat{\mathbf{w}} + \omega^2 \hat{\mathbf{w}} = 0 & \text{in } \Omega^{\text{PML}}, \\ \hat{\mathbf{w}}(x, b) = \mathbf{u}(x, b) & \text{on } \Gamma, \\ \hat{\mathbf{w}}(x, b + \delta) = 0 & \text{on } \Gamma^{\text{PML}}. \end{cases}$$

Using the definitions of the operators \mathcal{T}^{PML} and \mathcal{D} , we have

$$\mathcal{T}^{\text{PML}} \mathbf{u} = \mathcal{D} \hat{\mathbf{w}} \quad \text{on } \Gamma.$$

On the other hand, it follows from Green's formula and the extension that

$$\begin{aligned} \int_{\Gamma} \mathbf{u} \cdot \mathcal{D} \tilde{\mathbf{v}} dx &= \int_{\Gamma} \hat{\mathbf{w}} \cdot \mathcal{D} \tilde{\mathbf{v}} dx = - \int_{\Omega^{\text{PML}}} \left[\mu \nabla_{\hat{\mathbf{x}}} \tilde{\mathbf{v}} : \nabla_{\hat{\mathbf{x}}} \hat{\mathbf{w}} + (\lambda + \mu) (\nabla_{\hat{\mathbf{x}}} \cdot \tilde{\mathbf{v}}) (\nabla_{\hat{\mathbf{x}}} \cdot \hat{\mathbf{w}}) - \omega^2 \tilde{\mathbf{v}} \cdot \hat{\mathbf{w}} \right] dx \\ &= \int_{\Omega^{\text{PML}}} \left[\mu \Delta_{\hat{\mathbf{x}}} \hat{\mathbf{w}} + (\lambda + \mu) \nabla_{\hat{\mathbf{x}}} \nabla_{\hat{\mathbf{x}}} \cdot \hat{\mathbf{w}} + \omega^2 \hat{\mathbf{w}} \right] \cdot \tilde{\mathbf{v}} dx + \int_{\Gamma} \mathcal{D} \hat{\mathbf{w}} \cdot \tilde{\mathbf{v}} dx \\ &= \int_{\Gamma} \mathcal{D} \hat{\mathbf{w}} \cdot \tilde{\mathbf{v}} dx = \int_{\Gamma} \mathcal{T}^{\text{PML}} \mathbf{u} \cdot \tilde{\mathbf{v}} dx, \end{aligned}$$

which completes the proof. \square

Define $\mathring{H}_{\text{qp}}^1(D) = \{v \in H_{\text{qp}}^1(D) : v = 0 \text{ on } \Gamma^{\text{PML}}\}$. The following two lemmas are concerned with the stability of the extension. The proofs are given in Appendix.

Lemma 4.3. *Let $\mathbf{v} \in H_{\text{qp}}^1(\Omega)^2$ and $\tilde{\mathbf{v}} \in \mathring{H}_{\text{qp}}^1(D)^2$ be its extension satisfying (4.3). Then there exists a positive constant C_1 such that*

$$\|\nabla \tilde{\mathbf{v}}\|_{F(\Omega^{\text{PML}})} \leq \gamma_2 C_1 \|\mathbf{v}\|_{H^1(\Omega)^2},$$

Lemma 4.4. *Let $\mathbf{v} \in H_{\text{qp}}^1(\Omega)^2$ and $\tilde{\mathbf{v}} \in \mathring{H}_{\text{qp}}^1(D)^2$ be its extension satisfying (4.3). Then there exists a positive constant C_2 such that*

$$\|\mathcal{D}\tilde{\mathbf{v}}\|_{L^2(\Gamma^{\text{PML}})^2} \leq \gamma_2 C_2 \|\mathbf{v}\|_{H^1(\Omega)^2}.$$

For simplicity, we shall write $\tilde{\mathbf{v}}$ as \mathbf{v} in the rest of the paper since no confusion of the notation is incurred.

Lemma 4.5 (Error representation formula). *For any $\mathbf{v} \in H_{S,\text{qp}}^1(\Omega)^2$, which is extended to be a function in $H_{0,\text{qp}}^1(D)^2$ according to (4.3), and $\mathbf{v}_h \in \mathring{V}_h(D)^2$, we have*

$$\begin{aligned} a(\mathbf{u} - \hat{\mathbf{u}}_h, \mathbf{v}) &= - \int_D \mathbf{g} \cdot (\bar{\mathbf{v}} - \bar{\mathbf{v}}_h) d\mathbf{x} - b_D(\hat{\mathbf{u}}_h, \mathbf{v} - \mathbf{v}_h) \\ &\quad + \int_{\Gamma} (\mathcal{T} - \mathcal{T}^{\text{PML}})(\hat{\mathbf{u}}_h - \mathbf{u}_{\text{inc}}) \cdot \bar{\mathbf{v}} d\mathbf{x} + \int_{\Gamma^{\text{PML}}} (\Pi_h \mathbf{u}_{\text{inc}} - \mathbf{u}_{\text{inc}}) \cdot \mathcal{D}_{\hat{\mathbf{x}}} \bar{\mathbf{v}} d\mathbf{x}. \end{aligned}$$

Proof. It follows from (2.21) and (3.4) that

$$\begin{aligned} a(\mathbf{u} - \hat{\mathbf{u}}_h, \mathbf{v}) &= a(\mathbf{u} - \hat{\mathbf{u}}, \mathbf{v}) + a(\hat{\mathbf{u}} - \hat{\mathbf{u}}_h, \mathbf{v}) \\ &= \int_{\Gamma} (\mathcal{T} - \mathcal{T}^{\text{PML}})(\hat{\mathbf{u}} - \mathbf{u}_{\text{inc}}) \cdot \bar{\mathbf{v}} d\mathbf{x} + a^{\text{PML}}(\hat{\mathbf{u}} - \hat{\mathbf{u}}_h, \mathbf{v}) - \int_{\Gamma} (\mathcal{T} - \mathcal{T}^{\text{PML}})(\hat{\mathbf{u}} - \hat{\mathbf{u}}_h) \cdot \bar{\mathbf{v}} d\mathbf{x} \\ &= \int_{\Gamma} (\mathcal{T} - \mathcal{T}^{\text{PML}})(\hat{\mathbf{u}}_h - \mathbf{u}_{\text{inc}}) \cdot \bar{\mathbf{v}} d\mathbf{x} + a^{\text{PML}}(\hat{\mathbf{u}} - \hat{\mathbf{u}}_h, \mathbf{v}). \end{aligned}$$

Using (2.21) and Lemma 4.2 give

$$a^{\text{PML}}(\hat{\mathbf{u}} - \hat{\mathbf{u}}_h, \mathbf{v}) = b_{\Omega}(\hat{\mathbf{u}} - \hat{\mathbf{u}}_h, \mathbf{v}) - \int_{\Gamma} \mathcal{T}^{\text{PML}}(\hat{\mathbf{u}} - \hat{\mathbf{u}}_h) \cdot \mathbf{v} d\mathbf{x} = b_{\Omega}(\hat{\mathbf{u}} - \hat{\mathbf{u}}_h, \mathbf{v}) - \int_{\Gamma} (\hat{\mathbf{u}} - \hat{\mathbf{u}}_h) \cdot \mathcal{D}\bar{\mathbf{v}} d\mathbf{x}.$$

Since $\mathcal{L}\bar{\mathbf{v}} = 0$ in Ω^{PML} , we deduce by Green's formula that

$$b_{\Omega^{\text{PML}}}(\hat{\mathbf{u}} - \hat{\mathbf{u}}_h, \mathbf{v}) = - \int_{\Gamma} (\hat{\mathbf{u}} - \hat{\mathbf{u}}_h) \cdot \mathcal{D}\bar{\mathbf{v}} d\mathbf{x} + \int_{\Gamma^{\text{PML}}} (\hat{\mathbf{u}} - \hat{\mathbf{u}}_h) \cdot \mathcal{D}_{\hat{\mathbf{x}}} \bar{\mathbf{v}} d\mathbf{x}.$$

Applying (3.4) and (4.1) yields

$$\begin{aligned} a^{\text{PML}}(\hat{\mathbf{u}} - \hat{\mathbf{u}}_h, \mathbf{v}) &= b_D(\hat{\mathbf{u}} - \hat{\mathbf{u}}_h, \mathbf{v}) - \int_{\Gamma^{\text{PML}}} (\hat{\mathbf{u}} - \hat{\mathbf{u}}_h) \cdot \mathcal{D}_{\hat{\mathbf{x}}} \bar{\mathbf{v}} d\mathbf{x} \\ &= - \int_D \mathbf{g}(\bar{\mathbf{v}} - \bar{\mathbf{v}}_h) d\mathbf{x} - b_D(\hat{\mathbf{u}}_h, \mathbf{v} - \mathbf{v}_h) - \int_{\Gamma^{\text{PML}}} (\hat{\mathbf{u}} - \hat{\mathbf{u}}_h) \cdot \mathcal{D}_{\hat{\mathbf{x}}} \bar{\mathbf{v}} d\mathbf{x}, \end{aligned}$$

which completes the proof. \square

Clearly, it suffices to evaluate all the terms in the error representation formula in order to show the posteriori error estimate in the Theorem 4.1. Now we present the proof as follows.

Proof. Taking $\mathbf{v}_h = \Pi_h \mathbf{v}_h \in H_{0,\text{qp}}^1(D)^2$ in Lemma 4.5 for the error representation formula, we have

$$\begin{aligned} a(\mathbf{u} - \hat{\mathbf{u}}_h, \mathbf{v}) &= - \int_D \mathbf{g}(\bar{\mathbf{v}} - \bar{\mathbf{v}}_h) d\mathbf{x} - b_D(\hat{\mathbf{u}}_h, \mathbf{v} - \mathbf{v}_h) \\ &\quad + \int_{\Gamma} (\mathcal{T} - \mathcal{T}^{\text{PML}})(\hat{\mathbf{u}}_h - \mathbf{u}_{\text{inc}}) \cdot \bar{\mathbf{v}} d\mathbf{x} + \int_{\Gamma^{\text{PML}}} (\Pi_h \mathbf{u}_{\text{inc}} - \mathbf{u}_{\text{inc}}) \cdot \mathcal{D}_{\hat{\mathbf{x}}} \bar{\mathbf{v}} d\mathbf{x} \\ &= J_1 + J_2 + J_3 + J_4. \end{aligned}$$

-
- 1 Given the tolerance $\epsilon > 0, \tau \in (0, 1)$;
 - 2 Choose δ and σ such that $\hat{F}\Lambda^{1/2} \leq 10^{-8}$;
 - 3 Construct an initial triangulation \mathcal{M}_h over Ω and compute error estimators;
 - 4 While $\epsilon_h > \epsilon$ do
 - 5 choose $\hat{\mathcal{M}}_h \subset \mathcal{M}_h$ according to the strategy $\eta_{\hat{\mathcal{M}}_h} > \tau\eta_{\mathcal{M}_h}$;
 - 6 refine all the elements in $\hat{\mathcal{M}}_h$ and obtain a new mesh denoted still by \mathcal{M}_h ;
 - 7 solve the discrete problem (4.1) on the new mesh \mathcal{M}_h ;
 - 8 compute the corresponding error estimators;
 - 9 End while.
-

TABLE 1. The adaptive FEM algorithm.

It follows from integration by parts that

$$J_1 + J_2 = \sum_{T \in \mathcal{M}_h} \left(\int_T R_T \cdot (\bar{\mathbf{v}} - \Pi_h \bar{\mathbf{v}}) d\mathbf{x} + \sum_{e \subset \partial T} \frac{1}{2} \int_e J_e \cdot (\bar{\mathbf{v}} - \Pi_h \bar{\mathbf{v}}) d\mathbf{x} \right),$$

which gives after using the interpolation estimates and Lemma 4.3 that

$$|J_1 + J_2| \leq C \sum_{T \in \mathcal{M}_h} \eta_T \|\nabla \mathbf{v}\|_{F(\tilde{T})} \leq C(1 + \gamma_2 C_1) \left(\sum_{T \in \mathcal{M}_h} \eta_T^2 \right)^{1/2} \|\mathbf{v}\|_{H^1(\Omega)^2}.$$

By Lemmas 3.2 and 3.3, we obtain

$$|J_3| \leq \hat{F} \|\hat{\mathbf{u}}_h - \mathbf{u}_{\text{inc}}\|_{L^2(\Gamma)^2} \|\mathbf{v}\|_{L^2(\Gamma)^2} \leq \gamma_2 \hat{F} \|\hat{\mathbf{u}}_h - \mathbf{u}_{\text{inc}}\|_{L^2(\Gamma)^2} \|\mathbf{v}\|_{H^1(\Omega)^2}.$$

Finally, it follows from Lemmas 3.3 and 4.4 that

$$\begin{aligned} |J_4| &\leq C_2 \|\Pi_h \mathbf{u}_{\text{inc}} - \mathbf{u}_{\text{inc}}\|_{L^2(\Gamma^{\text{PML}})^2} \|\mathbf{v}\|_{L^2(\Gamma)^2} \\ &\leq \gamma_2 C_2 \|\Pi_h \mathbf{u}_{\text{inc}} - \mathbf{u}_{\text{inc}}\|_{L^2(\Gamma^{\text{PML}})^2} \|\mathbf{v}\|_{H^1(\Omega)^2}. \end{aligned}$$

The proof is completed by combining the above estimates □

5. NUMERICAL EXPERIMENTS

According to the discussion in section 3, we choose the PML medium property as the power function and need to specify the thickness δ of the layers and the medium parameter σ . Recall from Theorem 4.1 that the a posteriori error estimate consists of two parts: the PML error ϵ_{PML} and the finite element discretization error ϵ_{FEM} , where

$$\epsilon_{\text{PML}} = \hat{F} \|\mathbf{u}_h^{\text{PML}} - \mathbf{u}_{\text{inc}}\|_{L^2(\Gamma)^2}, \quad (5.1)$$

$$\epsilon_{\text{FEM}} = \|\mathbf{u}_h^{\text{PML}} - \mathbf{u}_{\text{inc}}\|_{L^2(\Gamma^{\text{PML}})^2} + \left(\sum_{T \in \mathcal{M}_h} \eta_T^2 \right)^{1/2}. \quad (5.2)$$

In our implementation, we first choose δ and σ such that $\hat{F}\Lambda^{1/2} \leq 10^{-8}$, which makes the PML error negligible compared with the finite element discretization error. Once the PML region and the medium property are fixed, we use the standard finite element adaptive strategy to modify the mesh according to the a posteriori error estimate (5.2). For any $T \in \mathcal{M}_h$, we define the local a posteriori error estimator

$$\hat{\eta}_T = \eta_T + \|\Pi_h \mathbf{u}_{\text{inc}} - \mathbf{u}_{\text{inc}}\|_{L^2(\Gamma^{\text{PML}} \cap \partial T)^2}.$$

The adaptive FEM algorithm is summarized in Table 1.

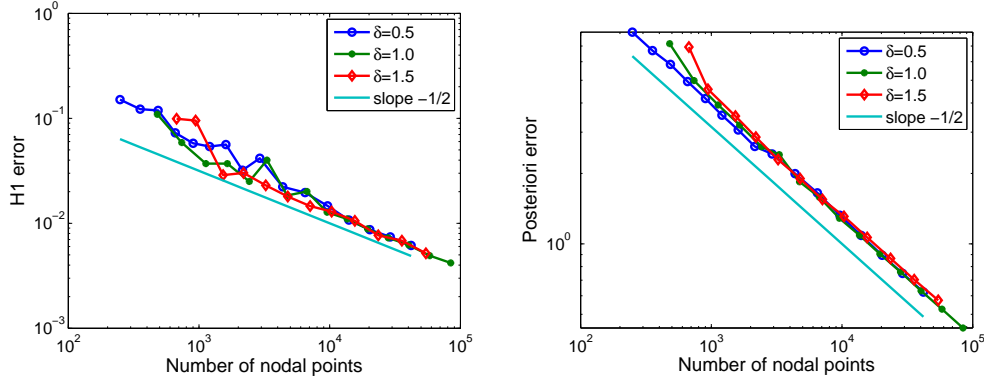


FIGURE 3. Example 1: Quasi-optimality of the a priori (left) and a posteriori (right) error estimates.

In the following, we present two examples to demonstrate the competitive numerical performance of the proposed algorithm. We choose $\lambda = 1$ and $\mu = 2$. The implementation of the adaptive algorithm is based on FreeFem++-cs [26].

Example 1. We consider the simplest periodic structure, a straight line. In this situation, the exact solution is available, which allows us to test the accuracy of the numerical algorithm. Assume that a plane compressional plane wave $\mathbf{u}_{\text{inc}} = [\sin \theta, -\cos \theta]^\top e^{i(\alpha x - \beta y)}$ is incident on the straight line $y = 0$, where $\alpha = \kappa_1 \sin \theta, \beta = \kappa_1 \cos \theta, \theta \in (-\pi/2, \pi/2)$ is the incident angle. It follows from the Navier equation, Helmholtz decomposition, and outgoing radiation condition that we obtain the exact solution

$$\mathbf{u}(x, y) = \mathbf{u}_{\text{inc}}(x, y) - [\alpha, \beta]^\top R_1 e^{i(\alpha x + \beta y)} - [\beta_2^{(0)}, -\alpha]^\top R_2 e^{i(\alpha x + \beta_2^{(0)} y)},$$

where $\beta_2^{(0)} = (\kappa_2^2 - \alpha^2)^{1/2}$ and

$$R_1 = \left(\frac{\alpha \sin \theta - \beta_2^{(0)} \cos \theta}{\alpha^2 + \beta \beta_2^{(0)}} \right), \quad R_2 = \left(\frac{\alpha \cos \theta + \beta \sin \theta}{\alpha^2 + \beta \beta_2^{(0)}} \right).$$

In our experiment, the parameters are chosen as $\theta = \pi/6, \omega = 2\pi$, and the domain $\Omega = (0, 1) \times (0, 1)$. Figure 3 shows the curves of $\log \|\nabla(\mathbf{u} - \hat{\mathbf{u}}_k)\|_{F(\Omega)}$ versus $\log N_k$ for both the a priori and the a posteriori error estimates, where N_k is the number of nodes of the mesh \mathcal{M}_k . The result shows that the meshes and the associated numerical complexity are quasi-optimal for the proposed method, i.e., $\log \|\nabla(\mathbf{u} - \hat{\mathbf{u}}_k)\|_{F(\Omega)} = C N_k^{-1/2}$ is valid asymptotically.

Example 2. This example is concerned with the scattering of the compressional plane wave $\mathbf{u}_{\text{inc}} = [\sin \theta, -\cos \theta]^\top e^{i(\alpha x - \beta y)}$ on a grating surface with a sharp angle. The problem geometry is shown in Figure 4. The parameters are chosen the same as those for Example 1. Since there is no exact solution for this example, we plot in Figure 5 the curves of $\log \|\nabla(\mathbf{u} - \hat{\mathbf{u}}_k)\|_{F(\Omega)}$ versus $\log N_k$ for the a posteriori error estimate, where N_k is the number of nodes of the mesh \mathcal{M}_k . Again, the result shows that the meshes and the associated numerical complexity are quasi-optimal for the proposed method. To verify Theorem 2.2, we plot in Figure 6 the grating efficiencies and the errors of the total efficiency for different PML thickness. Figure 7 shows the mesh and the amplitude of the associated solution after 6 adaptive iterations when the grating efficiency is stabilized. The mesh has 8491 nodes. This example shows clearly the ability of the proposed method to capture the singularity of the solution.

6. CONCLUDING REMARKS

We presented an adaptive finite element method with the PML absorbing layer technique for the elastic wave scattering problem in a periodic structure. We showed that the truncated PML problem has a unique weak solution which converges exponentially to the solution of the original problem by increasing the PML

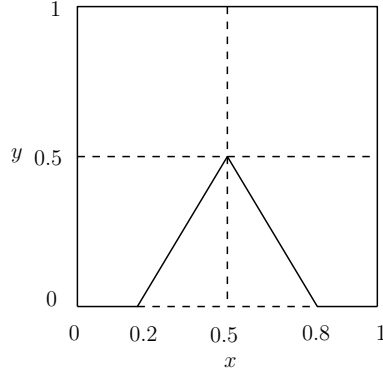


FIGURE 4. Example 2: Geometry of the domain

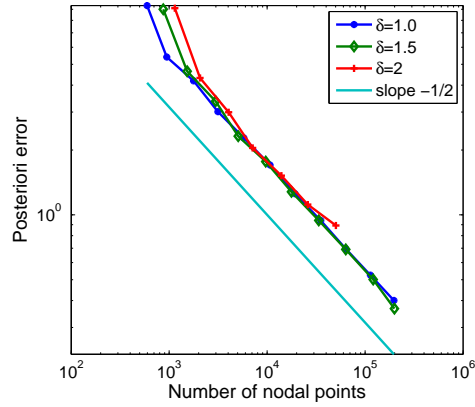
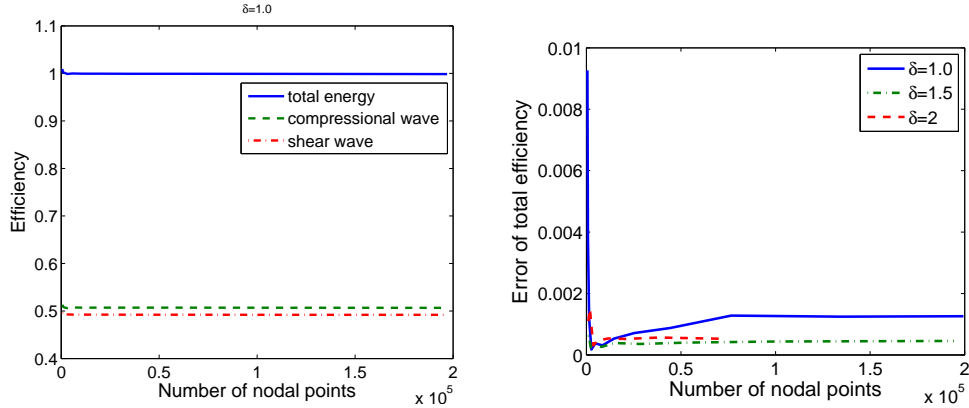


FIGURE 5. Example 2: Quasi-optimality of the a posteriori error estimates for different PML thickness.

FIGURE 6. Example 2: (left) Grating efficiency with $\delta = 1.0$; (right) Robustness of grating efficiency with respect to the thickness of PML layers

parameters. We deduced the a posteriori error estimate for the PML solution which serves as a basis for the adaptive finite element approximation. Numerical results show that the proposed method is effective to solve the diffractive grating problem of elastic waves. The method can be directly applied to solve the diffraction grating problems with other interface and/or boundary conditions. We are also currently extending the method to the three-dimensional problem where bi-periodic structures need to be considered.

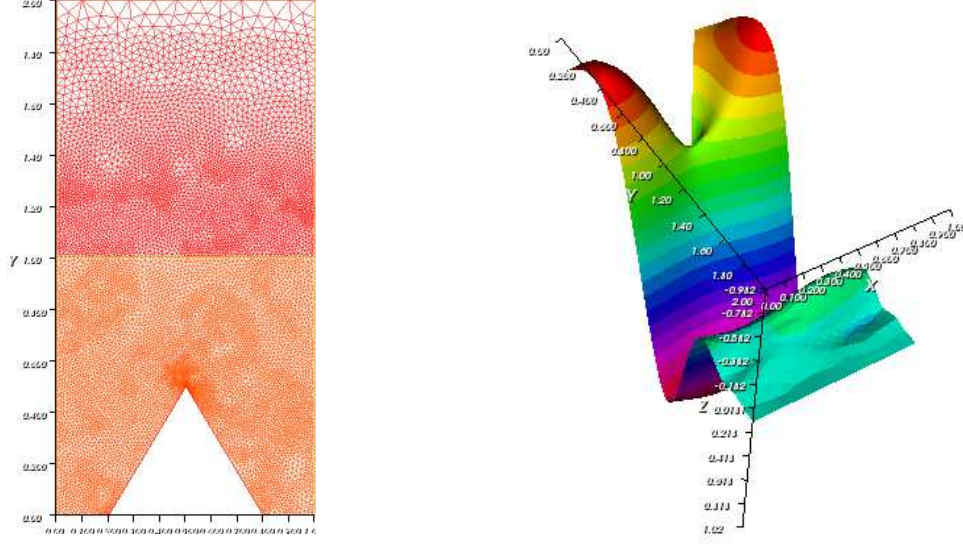


FIGURE 7. Example 2: The mesh (left) and the surface plot of the amplitude of the associated solution (right) after 6 adaptive iterations. The mesh has 8491 nodes.

APPENDIX A. TECHNICAL ESTIMATES

In this section, we present the proofs for some technical estimates which are used in our analysis for the error estimate between the solutions of the PML problem and the original scattering problem.

Proposition A.1. *For any $n \in \mathbb{Z}$, we have $\kappa_1^2 < |\chi^{(n)}| < \kappa_2^2$.*

Proof. Recalling (2.16) and (2.11), we consider three cases:

- (i) For $n \in U_1$, $\beta_1^{(n)} = (\kappa_1^2 - \alpha_n^2)^{1/2}$ and $\beta_2^{(n)} = (\kappa_2^2 - \alpha_n^2)^{1/2}$. We have

$$\chi^{(n)} = \alpha_n^2 + \beta_1^{(n)}\beta_2^{(n)} = \alpha_n^2 + (\kappa_1^2 - \alpha_n^2)^{1/2}(\kappa_2^2 - \alpha_n^2)^{1/2}.$$

Consider the function

$$g_1(t) = t + (k_1 - t)^{1/2}(k_2 - t)^{1/2}, \quad 0 < k_1 < k_2.$$

It is easy to know that g_1 is decreasing for $0 < t < k_1$. Hence

$$k_1 = g_1(k_1) < g_1(t) < g_1(0) = (k_1 k_2)^{1/2},$$

which gives $\kappa_1^2 < \chi^{(n)} < \kappa_1 \kappa_2$.

- (ii) For $n \in U_2 \setminus U_1$, $\beta_1^{(n)} = i(\alpha_n^2 - \kappa_1^2)^{1/2}$, $\beta_2^{(n)} = (\kappa_2^2 - \alpha_n^2)^{1/2}$. We have

$$\chi^{(n)} = \alpha_n^2 + i(\alpha_n^2 - \kappa_1^2)^{1/2}(\kappa_2^2 - \alpha_n^2)^{1/2}$$

and

$$|\chi^{(n)}|^2 = (\kappa_1^2 + \kappa_2^2)\alpha_n^2 - (\kappa_1 \kappa_2)^2,$$

which gives $\kappa_1^2 < |\chi^{(n)}| < \kappa_2^2$.

- (iii) For $n \notin U_2$, $\beta_1^{(n)} = i(\alpha_n^2 - \kappa_1^2)^{1/2}$, $\beta_2^{(n)} = i(\alpha_n^2 - \kappa_2^2)^{1/2}$. We have

$$\chi^{(n)} = \alpha_n^2 - (\alpha_n^2 - \kappa_1^2)^{1/2}(\alpha_n^2 - \kappa_2^2)^{1/2}.$$

Let

$$g_2(t) = t - (t - k_1)^{1/2}(t - k_2)^{1/2}, \quad 0 < k_1 < k_2.$$

It is easy to verify that the function g_2 is decreasing for $t > k_2$. Hence we have

$$(k_1 + k_2)/2 = g_2(\infty) < g_2(t) < g_2(k_2) = k_2,$$

which gives $(\kappa_1^2 + \kappa_2^2)/2 < \chi^{(n)} < \kappa_2^2$.

Combining the above estimates, we get $\kappa_1^2 < |\chi^{(n)}| < \kappa_2^2$ for any $n \in \mathbb{Z}$. \square

Proposition A.2. *The function $g_3(t) = t/(e^t - 1)$ is a decreasing function for $t > 0$.*

Proof. A simple calculation yields

$$g_3'(t) = \frac{(1-t)e^t - 1}{(e^t - 1)^2} < 0, \quad t > 0,$$

which completes the proof. \square

Proposition A.3. *The function $g_4(t) = t^k/e^{(t^2-s^2)^{1/2}/2}$ satisfies $g_4(t) \leq (s^2 + k^2)^{k/2}$ for any $t > s > 0$, $k \geq 2$.*

Proof. Using the change of variables $\tau = (t^2 - s^2)^{1/2}$, we have

$$\hat{g}_4(\tau) = \frac{(\tau^2 + s^2)^{k/2}}{e^{\tau/2}}.$$

Taking the derivative of \hat{g}_4 gives

$$\hat{g}_4'(\tau) = -\frac{(\tau^2 - k\tau + s^2)(\tau^2 + s^2)^{1/2}}{e^{\tau/2}}.$$

- (i) If $s \geq k/2$, then $\hat{g}_4' \leq 0$ for $\tau > 0$. The function \hat{g}_4 is decreasing and reaches its maximum at $\tau = 0$, i.e.,

$$g_4(t) \leq \hat{g}_4(0) = s^k.$$

- (ii) If $s < k/2$, then $\hat{g}_4' < 0$ for $\tau \in (0, (k - (k^2 - 4s^2)^{1/2})/2) \cup ((k + (k^2 - 4s^2)^{1/2})/2, \infty)$ and $\hat{g}_4 > 0$ for $\tau \in ((k - (k^2 - 4s^2)^{1/2})/2, (k + (k^2 - 4s^2)^{1/2})/2)$. Thus \hat{g}_4 reaches its maximum at either $\tau_1 = 0$ or $\tau_2 = (k + (k^2 - 4s^2)^{1/2})/2$. Thus we have

$$g_4(t) = \hat{g}_4(\tau) \leq \max\{\hat{g}_4(\tau_1), \hat{g}_4(\tau_2)\} \leq (s^2 + k^2)^{k/2}.$$

The proof is completed by combining the above estimates. \square

Proposition A.4. *For any $n \in \mathbb{Z}$, we have $\|M^{(n)} - \hat{M}^{(n)}\|_2 \leq \hat{F}$, where $\hat{F} = 17\omega^2 F/\kappa_1^4$.*

Proof. First, we have from (3.12) that

$$\begin{aligned} |\varepsilon_j^{(n)}| &= |\coth(-i\beta_j^{(n)}\zeta) - 1| = \frac{2}{|e^{-2i\beta_j^{(n)}\zeta} - 1|} \leq \frac{2}{|e^{-2i\beta_j^{(n)}\zeta}| - 1}, \\ |\delta_j^{(n)}| &= \left| \frac{e^{i\beta_2^{(n)}\zeta} - e^{i\beta_1^{(n)}\zeta}}{e^{-i\beta_j^{(n)}\zeta} - e^{i\beta_j^{(n)}\zeta}} \right| \leq \frac{2}{|e^{-i\beta_j^{(n)}\zeta}| - 1} = \frac{2}{e^{\text{Im}\beta_j^{(n)}\text{Re}\zeta + \text{Re}\beta_j^{(n)}\text{Im}\zeta} - 1}, \end{aligned}$$

and

$$|\varepsilon_1^{(n)}\eta^{(n)}| = \left| \frac{2e^{i\beta_1^{(n)}\zeta}}{e^{-i\beta_2^{(n)}\zeta} - e^{i\beta_2^{(n)}\zeta}} \right| \leq \frac{2}{|e^{-i\beta_2^{(n)}\zeta}| - 1}.$$

Thus we can take proper PML parameters σ and δ such that $|\delta_j^{(n)}| < 1$ for any $n \in \mathbb{Z}$.

Next we consider three cases:

- (i) For $n \in U_1$, we have $\beta_1^{(n)} = \Delta_1^{(n)}$, $\beta_2^{(n)} = \Delta_2^{(n)}$. Using the facts that $\Delta_j^{(n)} \geq \Delta_j^-$ for $n \in U_1$ and the function g_3 is decreasing for $t > 0$, we obtain from (2.16) and (3.13) that

$$|\hat{\chi}^{(n)} - \chi^{(n)}| \leq \frac{24\Delta_1^{(n)}\Delta_2^{(n)}}{|e^{-i\beta_1^{(n)}\zeta}| - 1} \leq \frac{12\kappa_2\Delta_1^-}{e^{\frac{1}{2}\Delta_1^-\text{Im}\zeta} - 1} \leq F,$$

and

$$\begin{aligned}
& \max \{ |\alpha_n(\hat{\chi}^{(n)} - \chi^{(n)})|, |\beta_1^{(n)}(\hat{\chi}^{(n)} - \chi^{(n)})|, |\beta_2^{(n)}(\hat{\chi}^{(n)} - \chi^{(n)})| \} \\
& \leq \frac{24\kappa_2^2 \Delta_1^{(n)}}{|e^{-i\beta_1^{(n)}\zeta} - 1|} \leq \frac{12\kappa_2^2 \Delta_1^-}{e^{\frac{1}{2}\Delta_1^- \text{Im}\zeta} - 1} \leq F, \\
& \max \{ |\varepsilon_1 \alpha_n^2 \beta_1^{(n)}|, |\varepsilon_1 \alpha_n \beta_1^{(n)} \beta_2^{(n)}|, |\varepsilon_1 \beta_1^{(n)} (\beta_2^{(n)})^2|, |\delta_1^{(n)} \alpha_n \beta_1^{(n)} \beta_2^{(n)}| \} \\
& \leq \frac{2\kappa_2^2 \Delta_1^{(n)}}{e^{2\Delta_1^{(n)} \text{Im}\zeta} - 1} \leq \frac{\kappa_2^2 \Delta_1^-}{e^{\Delta_1^- \text{Im}\zeta} - 1} \leq F, \\
& \max \left\{ |\varepsilon_1^{(n)} \eta^{(n)} \alpha_n \beta_1^{(n)} \beta_2^{(n)}|, |\varepsilon_1^{(n)} \eta^{(n)} \alpha_n^2 \beta_2^{(n)}|, |\delta_2^{(n)} \alpha_n^2 \beta_2^{(n)}|, \right. \\
& \quad \left. |\varepsilon_1^{(n)} \eta^{(n)} (\beta_1^{(n)})^2 \beta_2^{(n)}|, |\delta_2^{(n)} \alpha_n \beta_1^{(n)} \beta_2^{(n)}|, |\delta_2^{(n)} (\beta_1^{(n)})^2 \beta_2^{(n)}| \right\} \\
& \leq \frac{2\kappa_2^2 \Delta_2^{(n)}}{e^{\Delta_2^{(n)} \text{Im}\zeta} - 1} \leq \frac{\kappa_2^2 \Delta_2^-}{e^{\frac{1}{2}\Delta_2^- \text{Im}\zeta} - 1} \leq F.
\end{aligned}$$

(ii) For $n \in U_2 \setminus U_1$, we have $\beta_1^{(n)} = i\Delta_1(n)$, $\beta_2^{(n)} = \Delta_2^{(n)}$. Using the facts that $\Delta_1(n) \geq \Delta_1^+$, $\Delta_2^{(n)} \geq \Delta_2^-$ for $n \in U_2 \setminus U_1$ and the function g_3 is decreasing for $t > 0$ again, we get

$$\begin{aligned}
|\hat{\chi}^{(n)} - \chi^{(n)}| & \leq \frac{16\kappa_2^3}{\kappa_1^2} \frac{\Delta_2^{(n)}}{e^{\Delta_2^{(n)} \text{Im}\zeta} - 1} + \frac{8\kappa_2^3}{\kappa_1^2} \frac{\Delta_1^{(n)}}{e^{\Delta_1^{(n)} \text{Re}\zeta} - 1} \\
& \leq \frac{8\kappa_2^3}{\kappa_1^2} \frac{\Delta_2^-}{e^{\frac{1}{2}\Delta_2^- \text{Im}\zeta} - 1} + \frac{4\kappa_2^3}{\kappa_1^2} \frac{\Delta_1^+}{e^{\frac{1}{2}\Delta_1^+ \text{Re}\zeta} - 1} \leq F,
\end{aligned}$$

and

$$\begin{aligned}
& \max \{ |\alpha_n(\hat{\chi}^{(n)} - \chi^{(n)})|, |\beta_1^{(n)}(\hat{\chi}^{(n)} - \chi^{(n)})|, |\beta_2^{(n)}(\hat{\chi}^{(n)} - \chi^{(n)})| \} \\
& \leq \frac{16\kappa_2^4 \Delta_2^{(n)}}{e^{\Delta_2^{(n)} \text{Im}\zeta} - 1} + \frac{8\kappa_2^4 \Delta_1^{(n)}}{e^{\Delta_1^{(n)} \text{Re}\zeta} - 1} \leq \frac{8\kappa_2^4 \Delta_2^-}{e^{\frac{1}{2}\Delta_2^- \text{Im}\zeta} - 1} + \frac{4\kappa_2^4 \Delta_1^+}{e^{\frac{1}{2}\Delta_1^+ \text{Re}\zeta} - 1} \leq F, \\
& \max \{ |\varepsilon_1 \alpha_n^2 \beta_1^{(n)}|, |\varepsilon_1 \alpha_n \beta_1^{(n)} \beta_2^{(n)}|, |\varepsilon_1 \beta_1^{(n)} (\beta_2^{(n)})^2|, |\delta_1^{(n)} \alpha_n \beta_1^{(n)} \beta_2^{(n)}| \} \\
& \leq \frac{2\kappa_2^2 \Delta_1^{(n)}}{e^{2\Delta_1^{(n)} \text{Re}\zeta} - 1} \leq \frac{\kappa_2^2 \Delta_1^-}{e^{\Delta_1^- \text{Re}\zeta} - 1} \leq \frac{\kappa_2^2 \Delta_1^-}{e^{\frac{1}{2}\Delta_1^- \text{Re}\zeta} - 1} \leq F, \\
& \max \left\{ |\varepsilon_1^{(n)} \eta^{(n)} \alpha_n \beta_1^{(n)} \beta_2^{(n)}|, |\varepsilon_1^{(n)} \eta^{(n)} (\alpha_n)^2 \beta_2^{(n)}|, |\delta_2^{(n)} (\alpha_n)^2 \beta_2^{(n)}|, \right. \\
& \quad \left. |\varepsilon_1^{(n)} \eta^{(n)} (\beta_1^{(n)})^2 \beta_2^{(n)}|, |\delta_2^{(n)} \alpha_n \beta_1^{(n)} \beta_2^{(n)}|, |\delta_2^{(n)} (\beta_1^{(n)})^2 \beta_2^{(n)}| \right\} \\
& \leq \frac{2\kappa_2^2 \Delta_2^{(n)}}{e^{\Delta_2^{(n)} \text{Im}\zeta} - 1} \leq \frac{\kappa_2^2 \Delta_2^-}{e^{\frac{1}{2}\Delta_2^- \text{Im}\zeta} - 1} \leq F,
\end{aligned}$$

(iii) For $n \notin U_2$, we have $\beta_1^{(n)} = i\Delta_1^{(n)}$, $\beta_2^{(n)} = i\Delta_2^{(n)}$, and $\Delta_1^{(n)} > \Delta_2^{(n)}$. Noting $\text{Re}\zeta \geq 1$, we obtain

$$\begin{aligned}
|\hat{\chi}^{(n)} - \chi^{(n)}| & \leq \frac{24}{\kappa_1^2} \frac{|\alpha_n|^3 \Delta_2^{(n)}}{e^{\Delta_2^{(n)} \text{Re}\zeta} - 1} \leq \frac{24}{\kappa_1^2} \frac{|\alpha_n|^3}{e^{\frac{1}{2}\Delta_2^{(n)}}} \frac{\Delta_2^{(n)}}{e^{\frac{1}{2}\Delta_2^{(n)} \text{Re}\zeta} - 1} \\
& \leq \frac{24(9 + \kappa_2^2)^{3/2}}{\kappa_1^2} \frac{\Delta_1^+}{e^{\frac{1}{2}\Delta_1^+ \text{Re}\zeta} - 1} \leq F,
\end{aligned}$$

and

$$\begin{aligned}
& \max \left\{ |\alpha_n(\hat{\chi}^{(n)} - \chi^{(n)})|, |\beta_1^{(n)}(\hat{\chi}^{(n)} - \chi^{(n)})|, |\beta_2^{(n)}(\hat{\chi}^{(n)} - \chi^{(n)})| \right\} \\
& \leq \frac{24}{\kappa_1^2} \frac{|\alpha_n|^4 \Delta_2^{(n)}}{e^{\Delta_2^{(n)} \operatorname{Re} \zeta} - 1} \leq \frac{24}{\kappa_1^2} \frac{|\alpha_n|^4}{e^{\frac{1}{2} \Delta_2^{(n)}}} \frac{\Delta_2^{(n)}}{e^{\frac{1}{2} \Delta_2^{(n)} \operatorname{Re} \zeta} - 1} \leq \frac{24(16 + \kappa_2^2)^2}{\kappa_1^2} \frac{\Delta_1^+}{e^{\frac{1}{2} \Delta_1^+ \operatorname{Re} \zeta} - 1} \leq F, \\
& \max \left\{ |\varepsilon_1 \alpha_n^2 \beta_1^{(n)}|, |\varepsilon_1 \alpha_n \beta_1^{(n)} \beta_2^{(n)}|, |\varepsilon_1 \beta_1^{(n)} (\beta_2^{(n)})^2|, |\delta_1^{(n)} \alpha_n \beta_1^{(n)} \beta_2^{(n)}| \right\} \\
& \leq \frac{2\alpha_n^2 \Delta_1^{(n)}}{e^{2\Delta_1^{(n)} \operatorname{Re} \zeta} - 1} \leq \frac{2\alpha_n^2}{e^{\Delta_1^{(n)}}} \frac{\Delta_1^{(n)}}{e^{\Delta_1^{(n)} \operatorname{Re} \zeta} - 1} \leq 2(4 + \kappa_1^2) \frac{\Delta_1^+}{e^{\Delta_1^+ \operatorname{Re} \zeta} - 1} \leq F, \\
& \max \left\{ |\varepsilon_1^{(n)} \eta^{(n)} \alpha_n \beta_1^{(n)} \beta_2^{(n)}|, |\varepsilon_1^{(n)} \eta^{(n)} (\alpha_n)^2 \beta_2^{(n)}|, |\delta_2^{(n)} (\alpha_n)^2 \beta_2^{(n)}|, \right. \\
& \quad \left. |\varepsilon_1^{(n)} \eta^{(n)} (\beta_1^{(n)})^2 \beta_2^{(n)}|, |\delta_2^{(n)} \alpha_n \beta_1^{(n)} \beta_2^{(n)}|, |\delta_2^{(n)} (\beta_1^{(n)})^2 \beta_2^{(n)}| \right\} \\
& \leq \frac{2\alpha_n^2 \Delta_2^{(n)}}{e^{\Delta_2^{(n)} \operatorname{Re} \zeta} - 1} \leq \frac{2\alpha_n^2}{e^{\frac{1}{2} \Delta_2^{(n)}}} \frac{\Delta_2^{(n)}}{e^{\frac{1}{2} \Delta_2^{(n)} \operatorname{Re} \zeta} - 1} \leq 2(4 + \kappa_2^2) \frac{\Delta_2^+}{e^{\frac{1}{2} \Delta_2^+ \operatorname{Re} \zeta} - 1} \leq F,
\end{aligned}$$

where we have used the estimate for g_4 and the facts that $\Delta_j^{(n)} \geq \Delta_j^+$ for $n \notin U_2$ and g_3 is a decreasing function.

It follows from Proposition A.1 and the estimate $|\hat{\chi}^{(n)} - \chi^{(n)}| \leq F$ that $\kappa_1^2 - F \leq |\hat{\chi}^{(n)}| \leq \kappa_2^2 + F$. Again, we may choose some proper PML parameters σ and δ such that $F \leq \kappa_1^2/2$, which gives $|\hat{\chi}^{(n)}| \geq \kappa_1^2/2$.

Last, using the matrix norm and combining all the above estimates, we get

$$\begin{aligned}
\|M^{(n)} - \hat{M}^{(n)}\|_2^2 & \leq \frac{4\omega^4}{\kappa_1^8} \left(|\beta_1^{(n)}(\hat{\chi}^{(n)} - \chi^{(n)})|^2 + 2|\alpha_n(\hat{\chi}^{(n)} - \chi^{(n)})|^2 + |\beta_2^{(n)}(\hat{\chi}^{(n)} - \chi^{(n)})|^2 \right. \\
& + |\varepsilon_1^{(n)} \alpha_n^2 \beta_1^{(n)}|^2 + |\varepsilon_1^{(n)} \beta_1^{(n)} (\beta_2^{(n)})^2|^2 + 10|\varepsilon_1^{(n)} \alpha_n \beta_1^{(n)} \beta_2^{(n)}|^2 + |\varepsilon_1^{(n)} \eta^{(n)} (\beta_1^{(n)})^2 \beta_2^{(n)}|^2 \\
& + 2|\varepsilon_1^{(n)} \eta^{(n)} \alpha_n \beta_1^{(n)} \beta_2^{(n)}|^2 + |\varepsilon_1^{(n)} \eta^{(n)} \alpha_n^2 \beta_2^{(n)}|^2 + 4|\delta_2^{(n)} (\beta_1^{(n)})^2 \beta_2^{(n)}|^2 \\
& \left. + 16|\delta_1^{(n)} \alpha_n \beta_1^{(n)} \beta_2^{(n)}|^2 + 4|\delta_2^{(n)} \alpha_n^2 \beta_2^{(n)}|^2 + 24|\delta_2^{(n)} \alpha_n \beta_1^{(n)} \beta_2^{(n)}|^2 \right) \leq \frac{272\omega^4}{\kappa_1^8} F^2,
\end{aligned}$$

which completes the proof. \square

APPENDIX B. PROOF OF LEMMA 4.3

Let $\mathbf{w} = \bar{\mathbf{v}}$. The problem (4.3) can be written as

$$\begin{cases} \mu \Delta_{\hat{\mathbf{x}}} \mathbf{w} + (\lambda + \mu) \nabla_{\hat{\mathbf{x}}} \nabla_{\hat{\mathbf{x}}} \cdot \mathbf{w} + \omega^2 \mathbf{w} = 0 & \text{in } \Omega^{\text{PML}}, \\ \mathbf{w}(x, b) = \bar{\mathbf{v}}(x, b) & \text{on } \Gamma, \\ \mathbf{w}(x, b + \delta) = 0 & \text{on } \Gamma^{\text{PML}}. \end{cases} \quad (\text{B.1})$$

We introduce the Helmholtz decomposition to the solution of (B.1):

$$\mathbf{w} = \nabla_{\hat{\mathbf{x}}} \psi_1 + \operatorname{curl}_{\hat{\mathbf{x}}} \psi_2, \quad (\text{B.2})$$

where $\psi_j(\hat{\mathbf{x}})$ satisfies the Helmholtz equation

$$\Delta_{\hat{\mathbf{x}}} \psi_j + \kappa_j^2 \psi_j = 0. \quad (\text{B.3})$$

Due to the quasi-periodicity of the solution, we have the Fourier series expansion

$$\psi_j(x, y) = \sum_{n \in \mathbb{Z}} \psi_j^{(n)}(y) e^{-i\alpha_n x}. \quad (\text{B.4})$$

Substituting (B.4) into (B.3) yields

$$\rho^{-1} \frac{d}{dy} \left(\rho^{-1} \frac{d}{dy} \psi_j^{(n)}(y) \right) + (\beta_j^{(n)})^2 \psi_j^{(n)}(y) = 0. \quad (\text{B.5})$$

The general solutions of (B.5) is

$$\psi_j^{(n)}(y) = \tilde{A}_j^{(n)} e^{i\beta_j^{(n)} \int_b^y \rho(\tau) d\tau} + \tilde{B}_j^{(n)} e^{-i\beta_j^{(n)} \int_b^y \rho(\tau) d\tau}.$$

It follows from (B.2) that the coefficients $\tilde{A}_j^{(n)}$ and $\tilde{B}_j^{(n)}$ can be uniquely determined by solving the following linear equations

$$\begin{bmatrix} -\alpha_n & -\alpha_n & \beta_2^{(n)} & -\beta_2^{(n)} \\ \beta_1^{(n)} & -\beta_1^{(n)} & \alpha_n & \alpha_n \\ -\alpha_n e^{i\beta_1^{(n)} \zeta} & -\alpha_n e^{-i\beta_1^{(n)} \zeta} & \beta_2^{(n)} e^{i\beta_2^{(n)} \zeta} & -\beta_2^{(n)} e^{-i\beta_2^{(n)} \zeta} \\ \beta_1^{(n)} e^{i\beta_1^{(n)} \zeta} & -\beta_1^{(n)} e^{-i\beta_1^{(n)} \zeta} & \alpha_n e^{i\beta_2^{(n)} \zeta} & \alpha_n e^{-i\beta_2^{(n)} \zeta} \end{bmatrix} \begin{bmatrix} \tilde{A}_1^{(n)} \\ \tilde{B}_1^{(n)} \\ \tilde{A}_2^{(n)} \\ \tilde{B}_2^{(n)} \end{bmatrix} = \begin{bmatrix} -i\bar{v}_1^{(n)}(b) \\ -i\bar{v}_2^{(n)}(b) \\ 0 \\ 0 \end{bmatrix}. \quad (\text{B.6})$$

A straightforward calculation yields the solution of (B.6):

$$\begin{aligned} \tilde{A}_1^{(n)} &= \frac{i}{2\chi^{(n)} \hat{\chi}^{(n)}} \left\{ -\chi^{(n)} (\varepsilon_1^{(n)} + 2) (-\alpha_n \bar{v}_1^{(n)}(b) + \beta_2^{(n)} \bar{v}_2^{(n)}(b)) \right. \\ &\quad \left. + 2\beta_2^{(n)} (\varepsilon_1^{(n)} + 2\delta_1^{(n)}) (1 + \delta_2^{(n)} - \eta^{(n)}) (-\alpha_n \beta_1^{(n)} \bar{v}_1^{(n)}(b) + \alpha_n^2 \bar{v}_2^{(n)}(b)) \right\}, \\ \tilde{B}_1^{(n)} &= \frac{i}{2\chi^{(n)} \hat{\chi}^{(n)}} \left\{ \chi^{(n)} \varepsilon_1^{(n)} (-\alpha_n \bar{v}_1^{(n)}(b) - \beta_2^{(n)} \bar{v}_2^{(n)}(b)) \right. \\ &\quad \left. + 2(\varepsilon_1^{(n)} \delta_2^{(n)} + 2(\delta_1^{(n)} + \delta_1^{(n)} \delta_2^{(n)})) (-\alpha_n \beta_1^{(n)} \beta_2^{(n)} \bar{v}_1^{(n)}(b) - \alpha_n^2 \beta_2^{(n)} \bar{v}_2^{(n)}(b)) \right\}, \\ \tilde{A}_2^{(n)} &= \frac{i}{2\chi^{(n)} \hat{\chi}^{(n)}} \left\{ \chi^{(n)} [\varepsilon_1^{(n)} \eta^{(n)} - 2(\varepsilon_1^{(n)} + 1)(1 + \delta_2^{(n)})] (\beta_1^{(n)} \bar{v}_1^{(n)}(b) + \alpha_n \bar{v}_2^{(n)}(b)) \right. \\ &\quad \left. + 2\varepsilon_1^{(n)} (1 + \delta_2^{(n)} - \eta^{(n)}) ((\beta_1^{(n)})^2 \beta_2^{(n)} \bar{v}_1^{(n)}(b) + \alpha_n^3 \bar{v}_2^{(n)}(b)) \right\}, \\ \tilde{B}_2^{(n)} &= \frac{i}{2\chi^{(n)} \hat{\chi}^{(n)}} \left\{ \chi^{(n)} [2\delta_2^{(n)} (\varepsilon_1^{(n)} + 1) - \varepsilon_1^{(n)} \eta^{(n)}] (\beta_1^{(n)} \bar{v}_1^{(n)}(b) - \alpha_n \bar{v}_2^{(n)}(b)) \right. \\ &\quad \left. - 2\delta_2^{(n)} (\varepsilon_1^{(n)} + 2) ((\beta_1^{(n)})^2 \beta_2^{(n)} \bar{v}_1^{(n)}(b) - \alpha_n^3 \bar{v}_2^{(n)}(b)) \right\}. \end{aligned}$$

Noting $\tilde{\mathbf{v}} = \bar{\mathbf{w}}$ and using the Helmholtz decomposition (B.2) again, we obtain

$$\begin{aligned} \tilde{\mathbf{v}}(x, y) &= i \sum_{n \in \mathbb{Z}} \begin{bmatrix} \alpha_n \\ -\bar{\beta}_1^{(n)} \end{bmatrix} \tilde{A}_1^{(n)} e^{i(\alpha_n x - \bar{\beta}_1^{(n)} \int_b^y \bar{\rho}(\tau) d\tau)} + \begin{bmatrix} \alpha_n \\ \bar{\beta}_1^{(n)} \end{bmatrix} \tilde{B}_1^{(n)} e^{i(\alpha_n x + \bar{\beta}_1^{(n)} \int_b^y \bar{\rho}(\tau) d\tau)} \\ &\quad - \begin{bmatrix} \bar{\beta}_2^{(n)} \\ \alpha_n \end{bmatrix} \tilde{A}_2^{(n)} e^{i(\alpha_n x - \bar{\beta}_2^{(n)} \int_b^y \bar{\rho}(\tau) d\tau)} + \begin{bmatrix} \bar{\beta}_2^{(n)} \\ -\alpha_n \end{bmatrix} \tilde{B}_2^{(n)} e^{i(\alpha_n x + \bar{\beta}_2^{(n)} \int_b^y \bar{\rho}(\tau) d\tau)}. \quad (\text{B.7}) \end{aligned}$$

Using the orthogonality of the Fourier modes in (B.7), we have

$$\begin{aligned} \int_0^\Lambda (|\partial_x \tilde{v}_1|^2 + |\partial_x \tilde{v}_2|^2 + |\partial_y \tilde{v}_1|^2 + |\partial_y \tilde{v}_2|^2) dx \leq 2\Lambda \sum_{n \in \mathbb{Z}} & \left[|\alpha_n^2 \bar{A}_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}|^2 + |\alpha_n^2 \bar{B}_1^{(n)} e^{i\beta_1^{(n)} \hat{y}}|^2 \right. \\ & + |\alpha_n \beta_2^{(n)} \bar{A}_2^{(n)} e^{-i\beta_2^{(n)} \hat{y}}|^2 + |\alpha_n \beta_2^{(n)} \bar{B}_2^{(n)} e^{i\beta_2^{(n)} \hat{y}}|^2 + |\alpha_n \beta_1^{(n)} \bar{A}_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}|^2 \\ & + |\alpha_n \beta_1^{(n)} \bar{B}_1^{(n)} e^{i\beta_1^{(n)} \hat{y}}|^2 + |\alpha_n^2 \bar{A}_2^{(n)} e^{-i\beta_2^{(n)} \hat{y}}|^2 + |\alpha_n^2 \bar{B}_2^{(n)} e^{i\beta_2^{(n)} \hat{y}}|^2 + |\alpha_n \beta_1^{(n)} \bar{A}_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}|^2 \\ & + |\alpha_n \beta_1^{(n)} \bar{B}_1^{(n)} e^{i\beta_1^{(n)} \hat{y}}|^2 + |(\beta_2^{(n)})^2 \bar{A}_2^{(n)} e^{-i\beta_1^{(n)} \hat{y}}|^2 + |(\beta_2^{(n)})^2 \bar{B}_2^{(n)} e^{i\beta_1^{(n)} \hat{y}}|^2 + |(\beta_1^{(n)})^2 \bar{A}_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}|^2 \\ & \left. + |(\beta_1^{(n)})^2 \bar{B}_1^{(n)} e^{i\beta_1^{(n)} \hat{y}}|^2 + |\alpha_n \beta_2^{(n)} \bar{A}_2^{(n)} e^{-i\beta_1^{(n)} \hat{y}}|^2 + |\alpha_n \beta_2^{(n)} \bar{B}_2^{(n)} e^{i\beta_1^{(n)} \hat{y}}|^2 \right]. \end{aligned}$$

We may pick some appropriate PML parameters σ and δ such that $|\chi^{(n)} - \hat{\chi}^{(n)}| \leq \kappa_1^2/2$ and $|\hat{\chi}^{(n)}| \geq \kappa_1^2/2$. It follows from the definition of $\bar{A}_1^{(n)}$ that

$$\begin{aligned} |\alpha_n^2 \bar{A}_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| & \leq \frac{|\alpha_n|}{\kappa_1^8} \left\{ \kappa_2^4 |\alpha_n|^5 |\varepsilon_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}|^2 + 4|\alpha_n|^5 |(\varepsilon_1^{(n)} \delta_2^{(n)} + 2(\delta_1^{(n)} + \delta_1^{(n)} \delta_2^{(n)})) \right. \\ & \quad \times \beta_1^{(n)} \beta_2^{(n)} e^{-i\beta_1^{(n)} \hat{y}}|^2 \Big\} |v_1^{(n)}(b)|^2 + \frac{|\alpha_n|}{\kappa_1^8} \left\{ \kappa_2^4 |\alpha_n|^5 |\varepsilon_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}|^2 \right. \\ & \quad \left. + 4|\alpha_n|^7 |(\varepsilon_1^{(n)} \delta_2^{(n)} + 2(\delta_1^{(n)} + \delta_1^{(n)} \delta_2^{(n)})) \beta_2^{(n)} e^{-i\beta_1^{(n)} \hat{y}}|^2 \right\} |v_2^{(n)}(b)|^2. \end{aligned} \quad (\text{B.8})$$

Since the estimates are similar for the coefficients in front of $v_1^{(n)}(b)$ and $v_2^{(n)}(b)$ in (B.8), we just present the estimates for the coefficients in front of $v_1^{(n)}(b)$.

Again, it is necessary to consider three cases:

(i) If $n \in U_1$, we have $\beta_1^{(n)} = \Delta_1^{(n)}$, $\beta_2^{(n)} = \Delta_2^{(n)}$, $\Delta_1^{(n)} < \Delta_2^{(n)}$, $|\alpha_n| \leq \kappa_1$, $|\beta_1^{(n)}| \leq \kappa_1$, $|\beta_2^{(n)}| \leq \kappa_2$, and

$$\begin{aligned} |\alpha_n|^{5/2} |\varepsilon_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| & \leq \frac{2\kappa_1^{5/2} e^{\Delta_1^{(n)} \text{Im} \hat{y} - \text{Im} \zeta}}{e^{\Delta_1^{(n)} \text{Im} \zeta} - 1} \leq \frac{2\kappa_1^{5/2}}{e^{\Delta_1^- \text{Im} \zeta} - 1}, \\ |\alpha_n|^{5/2} |\beta_1^{(n)} \beta_2^{(n)}| |\varepsilon_1^{(n)} \delta_2^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| & \leq \frac{2\kappa_1^{7/2} \kappa_2 e^{-\Delta_1^{(n)} \text{Im} \zeta}}{e^{\Delta_1^{(n)} \text{Im} \zeta} - 1} \frac{2}{e^{\Delta_2^{(n)} \text{Im} \zeta} - 1} e^{\Delta_1^{(n)} \text{Im} \hat{y}} \\ & \leq \frac{4\kappa_1^{7/2} \kappa_2}{(e^{\Delta_1^- \text{Im} \zeta} - 1)(e^{\Delta_2^- \text{Im} \zeta} - 1)}, \\ |\alpha_n|^{5/2} |\beta_1^{(n)} \beta_2^{(n)}| |\delta_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| & \leq \frac{2\kappa_1^{7/2} \kappa_2 (e^{-\Delta_2^{(n)} \text{Im} \zeta} + e^{-\Delta_1^{(n)} \text{Im} \zeta})}{e^{\Delta_1^{(n)} \text{Im} \zeta} - 1} e^{\Delta_1^{(n)} \text{Im} \hat{y}} \\ & \leq \frac{4\kappa_1^{7/2} \kappa_2}{e^{\Delta_1^- \text{Im} \zeta} - 1}, \\ |\alpha_n|^{5/2} |\beta_1^{(n)} \beta_2^{(n)}| |\delta_1^{(n)} \delta_2^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| & \leq |\alpha_n|^{5/2} |\beta_1^{(n)} \beta_2^{(n)} \delta_2^{(n)}| |\delta_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| \\ & \leq \frac{8\kappa_1^{7/2} \kappa_2}{(e^{\Delta_1^- \text{Im} \zeta} - 1)(e^{\Delta_2^- \text{Im} \zeta} - 1)}. \end{aligned}$$

(ii) If $n \in U_2 \setminus U_1$, we have $\beta_1^{(n)} = i\Delta_1^{(n)}$, $\beta_2^{(n)} = \Delta_2^{(n)}$, $|\alpha_n| \leq \kappa_2$, $\Delta_j^{(n)} \leq \kappa_2$, and

$$|\alpha_n|^{5/2} |\varepsilon_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| \leq \frac{2\kappa_2^{5/2} e^{\Delta_1^{(n)} (\text{Re} \hat{y} - \text{Re} \zeta)}}{e^{\Delta_1^{(n)} \text{Re} \zeta} - 1} \leq \frac{2\kappa_2^{5/2}}{e^{\Delta_1^+ \text{Re} \zeta} - 1},$$

$$\begin{aligned}
|\alpha_n|^{5/2} |\beta_1^{(n)} \beta_2^{(n)}| |\varepsilon_1^{(n)} \delta_2^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| &\leq \frac{2\kappa_2^{9/2} e^{-\Delta_1^{(n)} \operatorname{Re} \zeta}}{e^{\Delta_1^{(n)} \operatorname{Re} \zeta} - 1} \frac{2}{e^{\Delta_2^{(n)} \operatorname{Im} \zeta} - 1} e^{\Delta_1^{(n)} \operatorname{Re} \hat{y}} \\
&\leq \frac{4\kappa_2^{9/2}}{(e^{\Delta_1^+ \operatorname{Re} \zeta} - 1)(e^{\Delta_2^- \operatorname{Im} \zeta} - 1)},
\end{aligned}$$

$$\begin{aligned}
|\alpha_n|^{5/2} |\beta_1^{(n)} \beta_2^{(n)}| |\delta_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| &\leq \frac{2\kappa_2^{9/2}}{e^{\Delta_1^{(n)} \operatorname{Re} \zeta} - 1} e^{\Delta_1^{(n)} \operatorname{Re} \hat{y}} \\
&\leq \frac{2\kappa_2^{9/2} e^{\Delta_1^{(n)} \operatorname{Re} \zeta}}{e^{\Delta_1^{(n)} \operatorname{Re} \zeta} - 1} \leq \frac{2\kappa_2^{9/2} e^{\Delta_1^+ \operatorname{Re} \zeta}}{e^{\Delta_1^+ \operatorname{Re} \zeta} - 1},
\end{aligned}$$

$$\begin{aligned}
|\alpha_n|^{5/2} |\beta_1^{(n)} \beta_2^{(n)}| |\delta_1^{(n)} \delta_2^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| &\leq |\alpha_n|^{5/2} |\beta_1^{(n)} \beta_2^{(n)} \delta_2^{(n)}| |\delta_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| \\
&\leq \frac{4\kappa_2^{9/2} e^{\Delta_1^+ \operatorname{Re} \zeta}}{(e^{\Delta_1^+ \operatorname{Re} \zeta} - 1)(e^{\Delta_2^- \operatorname{Im} \zeta} - 1)}.
\end{aligned}$$

(iii) If $n \notin U_2$, we have $\beta_1^{(n)} = i\Delta_1^{(n)}$, $\beta_2^{(n)} = i\Delta_2^{(n)}$, $\Delta_2^{(n)} < \Delta_1^{(n)} \leq |\alpha_n|$, and

$$\begin{aligned}
|\alpha_n|^{5/2} |\varepsilon_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| &\leq \frac{2|\alpha_n|^{5/2} e^{\Delta_1^{(n)} (\operatorname{Re} \hat{y} - \operatorname{Re} \zeta)}}{e^{\Delta_1^{(n)} \operatorname{Re} \zeta} - 1} \leq \frac{2|\alpha_n|^{5/2}}{e^{\frac{1}{2}\Delta_1^{(n)}}} \frac{1}{e^{\frac{1}{2}\Delta_1^+ \operatorname{Re} \zeta} - 1} \\
&\leq \frac{2(\kappa_1^2 + 25/4)^{5/4}}{e^{\frac{1}{2}\Delta_1^+ \operatorname{Re} \zeta} - 1},
\end{aligned}$$

$$\begin{aligned}
|\alpha_n|^{5/2} |\beta_1^{(n)} \beta_2^{(n)}| |\varepsilon_1^{(n)} \delta_2^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| &\leq |\alpha_n|^{9/2} |\varepsilon_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| |\delta_2^{(n)}| \\
&\leq \frac{4(\kappa_1^2 + 81/4)^{9/4}}{(e^{\frac{1}{2}\Delta_1^+ \operatorname{Re} \zeta} - 1)(e^{\Delta_2^+ \operatorname{Re} \zeta} - 1)},
\end{aligned}$$

$$\begin{aligned}
|\alpha_n|^{5/2} |\beta_1^{(n)} \beta_2^{(n)}| |\delta_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| &\leq \frac{|\alpha_n|^{9/2} (e^{-\Delta_2^{(n)} \operatorname{Re} \zeta} + e^{-\Delta_1^{(n)} \operatorname{Re} \zeta})}{e^{\Delta_1^{(n)} \operatorname{Re} \zeta} - 1} e^{\Delta_1^{(n)} \operatorname{Re} \hat{y}} \\
&\leq \frac{2|\alpha_n|^{9/2}}{e^{\Delta_1^{(n)} \operatorname{Re} \zeta} - 1} \leq \frac{2(\kappa_1^2 + 81/4)^{9/4}}{e^{\frac{1}{2}\Delta_1^+ \operatorname{Re} \zeta} - 1},
\end{aligned}$$

$$\begin{aligned}
|\alpha_n|^{5/2} |\beta_1^{(n)} \beta_2^{(n)}| |\delta_1^{(n)} \delta_2^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| &\leq |\alpha_n|^{5/2} |\beta_1^{(n)} \beta_2^{(n)} \delta_2^{(n)}| |\delta_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}| \\
&\leq \frac{4(\kappa_1^2 + 81/4)^{9/4}}{(e^{\frac{1}{2}\Delta_1^+ \operatorname{Re} \zeta} - 1)(e^{\Delta_2^+ \operatorname{Re} \zeta} - 1)}.
\end{aligned}$$

We have used Proposition (A.3) in the above estimates. Combining these estimates, we may obtain

$$|\alpha_n^2 \tilde{A}_1^{(n)} e^{-i\beta_1^{(n)} \hat{y}}|^2 \leq C |\alpha_n| (|v_1^{(n)}|^2 + |v_2^{(n)}|^2),$$

where the positive real number C_1 depends on κ_j , Δ_j^- , Δ_j^+ , $\operatorname{Re} \zeta$, and $\operatorname{Im} \zeta$. Following from a similar argument with tedious calculations yields

$$\|\nabla \tilde{\mathbf{v}}\|_{F(\Omega^{\text{PML}})}^2 \leq C_1 \Lambda \sum_{n \in \mathbb{Z}} |\alpha_n| (|v_1^{(n)}|^2 + |v_2^{(n)}|^2),$$

where we have used the fact $|\beta_j^{(n)}| \leq C(1 + |\alpha_n|)$ for $n \in \mathbb{Z}$. Finally, we have from Lemma 3.3 that

$$\|\nabla \tilde{\mathbf{v}}\|_{F(\Omega^{\text{PML}})} \leq C_1 \|\mathbf{v}\|_{H^{1/2}(\Gamma)^2} \leq \gamma_2 C_1 \|\mathbf{v}\|_{H^1(\Omega)^2},$$

which completes the proof.

APPENDIX C. PROOF OF LEMMA 4.4

Taking the complex conjugate of (B.7) and using (2.18), we have

$$\begin{aligned} \mathcal{D}\tilde{\mathbf{v}}(x, b + \delta) = & - \sum_{n \in \mathbb{Z}} \left[\frac{-\mu\rho\alpha_n\beta_1^{(n)}}{(\lambda + \mu)\alpha_n^2 + (\lambda + 2\mu)\bar{\rho}(\beta_1^{(n)})^2} \right] \tilde{A}_1^{(n)} e^{-i(\alpha_n x - \beta_1^{(n)}\zeta)} \\ & + \left[\frac{\mu\rho\alpha_n\beta_1^{(n)}}{(\lambda + \mu)\alpha_n^2 + (\lambda + 2\mu)\rho(\beta_1^{(n)})^2} \right] \tilde{B}_1^{(n)} e^{-i(\alpha_n x + \beta_1^{(n)}\zeta)} \\ & + \left[\frac{\mu\rho(\beta_2^{(n)})^2}{-(\lambda + \mu)\alpha_n\beta_2^{(n)} + (\lambda + 2\mu)\rho\alpha_n\beta_2^{(n)}} \right] \tilde{A}_2^{(n)} e^{-i(\alpha_n x - \beta_2^{(n)}\zeta)} \\ & + \left[\frac{\mu\rho\alpha_n(\beta_2^{(n)})^2}{(\lambda + \mu)\alpha_n\beta_2^{(n)} - (\lambda + 2\mu)\rho\alpha_n\beta_2^{(n)}} \right] \tilde{B}_2^{(n)} e^{-i(\alpha_n x + \beta_2^{(n)}\zeta)}. \end{aligned}$$

A straightforward calculation yields that

$$\begin{aligned} \|\mathcal{D}\tilde{\mathbf{v}}(x, b + \delta)\|_{L^2(\Gamma^{\text{PML}})^2}^2 = & \|\mathcal{D}\tilde{\mathbf{v}}(x, b + \delta)\|_{L^2(\Gamma^{\text{PML}})^2}^2 \leq 2\Lambda \sum_{n \in \mathbb{Z}} \left(|\mu\rho\alpha_n\beta_1^{(n)} \tilde{A}_1^{(n)} e^{i\beta_1^{(n)}\zeta}|^2 \right. \\ & + |\mu\rho\alpha_n\beta_1^{(n)} \tilde{B}_1^{(n)} e^{-i\beta_1^{(n)}\zeta}|^2 + |\mu\rho(\beta_2^{(n)})^2 \tilde{A}_2^{(n)} e^{i\beta_2^{(n)}\zeta}|^2 + |\mu\rho(\beta_2^{(n)})^2 \tilde{B}_2^{(n)} e^{-i\beta_2^{(n)}\zeta}|^2 \\ & + |((\lambda + \mu)\alpha_n^2 + (\lambda + 2\mu)\rho(\beta_1^{(n)})^2) \tilde{A}_1^{(n)} e^{i\beta_1^{(n)}\zeta}|^2 + |((\lambda + \mu)\alpha_n^2 + (\lambda + 2\mu)\rho(\beta_1^{(n)})^2) \tilde{B}_1^{(n)} e^{-i\beta_1^{(n)}\zeta}|^2 \\ & \left. + |((\lambda + \mu)\alpha_n\beta_2^{(n)} - (\lambda + 2\mu)\rho\alpha_n\beta_2^{(n)}) \tilde{A}_2^{(n)} e^{i\beta_2^{(n)}\zeta}|^2 + |((\lambda + \mu)\alpha_n\beta_2^{(n)} - (\lambda + 2\mu)\rho\alpha_n\beta_2^{(n)}) \tilde{B}_2^{(n)} e^{-i\beta_2^{(n)}\zeta}|^2 \right). \end{aligned}$$

Using the similar technique in the proof of Lemma 4.3 and omitting the details, we may show that there exists a positive constant C_2 such that

$$\|\mathcal{D}\tilde{\mathbf{v}}(x, b + \delta)\|_{L^2(\Gamma^{\text{PML}})^2}^2 \leq C_2 \sum_{n \in \mathbb{Z}} [(1 + |\alpha_n|)(|v_1^{(n)}(b)|^2 + |v_1^{(n)}(b)|^2)].$$

Finally, it follows from Lemma 3.3 that

$$\|\mathcal{D}\tilde{\mathbf{v}}(x, b + \delta)\|_{L^2(\Gamma^{\text{PML}})^2} \leq C_2 \|\mathbf{v}\|_{H^{1/2}(\Gamma)^2} \leq \gamma_2 C_2 \|\mathbf{v}\|_{H^1(\Omega)^2},$$

which completes the proof.

REFERENCES

- [1] T. Arens, The scattering of plane elastic waves by a one-dimensional periodic surface, *Math. Methods Appl. Sci.*, 22 (1999), 55–72.
- [2] T. Arens, A new integral equation formulation for the scattering of plane elastic waves by diffraction gratings, *J. Integral Equations Applications*, 11 (1999), 275–297.
- [3] I. Babuška and A. Aziz, Survey Lectures on Mathematical Foundations of the Finite Element Method, in *The Mathematical Foundations of the Finite Element Method with Application to the Partial Differential Equations*, ed. by A. Aziz, Academic Press, New York, 1973, 5–359.
- [4] G. Bao, Finite element approximation of time harmonic waves in periodic structures, *SIAM J. Numer. Anal.*, 32 (1995), 1155–1169.
- [5] G. Bao, Variational approximation of Maxwells equations in biperiodic structures, *SIAM J. Appl. Math.*, 57 (1997), 364–381.
- [6] G. Bao, Z. Chen, and H. Wu, Adaptive finite element method for diffraction gratings, *J. Opt. Soc. Amer. A*, 22 (2005), 1106–1114.
- [7] G. Bao, D. C. Dobson, and J. A. Cox, Mathematical studies in rigorous grating theory, *J. Opt. Soc. Amer. A*, 12 (1995), 1029–1042.
- [8] G. Bao, L. Cowsar, and W. Masters, eds., *Mathematical Modeling in Optical Science*, *Frontiers Appl. Math.*, 22, SIAM, Philadelphia, 2001.

- [9] G. Bao, P. Li, and H. Wu, An adaptive edge element method with perfectly matched absorbing layers for wave scattering by periodic structures, *Math. Comp.*, 79 (2010), 1–34.
- [10] G. Bao and H. Wu, On the convergence of the solutions of PML equations for Maxwell’s equations, *SIAM J. Numer. Anal.*, 43 (2005), 2121–2143.
- [11] J.-P. Bérenger, A perfectly matched layer for the absorption of electromagnetic waves, *J. Comput. Phys.*, 114 (1994), 185–200.
- [12] J. H. Bramble and J. E. Pasciak, Analysis of a finite PML approximation for the three dimensional time-harmonic Maxwell and acoustic scattering problems, *Math. Comp.*, 76 (2007), 597–614.
- [13] J. H. Bramble, J. E. Pasciak, and D. Trenev, Analysis of a finite PML approximation to the three dimensional elastic wave scattering problem, *Math. Comp.*, 79 (2010), 2079–2101.
- [14] J. Chen and Z. Chen, An adaptive perfectly matched layer technique for 3-D time-harmonic electromagnetic scattering problems, *Math. Comp.*, 77 (2008), 673–698.
- [15] X. Chen and A. Friedman, Maxwell’s equations in a periodic structure, *Trans. Amer. Math. Soc.*, 323 (1991), 4650–507.
- [16] Z. Chen and H. Wu, An adaptive finite element method with perfectly matched absorbing layers for the wave scattering by periodic structures, *SIAM J. Numer. Anal.*, 41 (2003), 799–826.
- [17] Z. Chen and X. Liu, An adptive perfectly matched layer technique for time-harmonic scattering problems, *SIAM J. Numer. Anal.*, 43 (2005), 645–671.
- [18] Z. Chen, X. Xiang, and X. Zhang, Convergence of the PML method for elastic wave scattering problems, *Math. Comp.*, to appear.
- [19] F. Collino and P. Monk, The perfectly matched layer in curvilinear coordinates, *SIAM J. Sci. Comput.*, 19 (1998), 2061–1090.
- [20] F. Collino and C. Tsogka, Application of the perfectly matched absorbing layer model to the linear elastodynamic problem in anisotropic heterogeneous media, *Geophysics*, 66 (2001), 294–307.
- [21] W. Chew and W. Weedon, A 3D perfectly matched medium for modified Maxwell’s equations with stretched coordinates, *Microwave Opt. Techno. Lett.*, 13 (1994), 599–604.
- [22] D. Dobson and A. Friedman, The time-harmonic Maxwell equations in a doubly periodic structure, *J. Math. Anal. Appl.*, 166 (1992), 507–528.
- [23] J. Elschner and G. Hu, Variational approach to scattering of plane elastic waves by diffraction gratings, *Math. Meth. Appl. Sci.*, 33 (2010), 1924–1941.
- [24] J. Elschner and G. Hu, Scattering of plane elastic waves by three-dimensional diffraction gratings, *Math. Models Methods Appl. Sci.*, 22 (2012), 1150019.
- [25] F. D. Hastings, J. B. Schneider, and S. L. Broschat, Application of the perfectly matched layer (PML) absorbing boundary condition to elastic wave propagation, *J. Acoust. Soc. Am.*, 100 (1996), 3061–3069.
- [26] F. Hecht, New development in FreeFem++, *J. Numer. Math.*, 20 (2012), 251–265.
- [27] T. Hohage, F. Schmidt, and L. Zschiedrich, Solving time-harmonic scattering problems based on the pole condition. II: Convergence of the PML method, *SIAM J. Math. Anal.*, 35 (2003), 547–560.
- [28] M. Lassas and E. Somersalo, On the existence and convergence of the solution of PML equations, *Computing*, 60 (1998), 229–241.
- [29] P. Li, Y. Wang, and Y. Zhao, Inverse elastic surface scattering with near-field data, *Inverse Problems*, 31 (2015), 035009.
- [30] A. H. Schatz, An observation concerning Ritz-Galerkin methods with indefinite bilinear forms, *Math. Comp.*, 28 (1974), 959–962.
- [31] E. Turkel and A. Yefet, Absorbing PML boundary layers for wave-like equations, *Appl. Numer. Math.*, 27 (1998), 533–557.
- [32] Z. Wang, G. Bao, J. Li, P. Li, and H. Wu, An adaptive finite element method for the diffraction grating problem with transparent boundary condition, *SIAM J. Numer. Anal.*, 53 (2015), 1585–1607.

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